



**S5P/TROPOMI Level 2
Product Format Specification
for the
offline Total Bromine Monoxide algorithm
TCBRO
and its auxiliary algorithm BGBRO**



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		Through out	Adaptations in relation to the dynamic treatment of the file class. The default file class is "OFFL".
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1 Introduction

1.1 Identification

This document describes in detail the structure and content of the Level-2 (L2) file products as generated by the S-5P TCBRO algorithm for the offline retrieval of total vertical BrO columns and of its auxiliary processor BGBRO for the offline derivation of reference spectral data and slant column background correction parameters. TCBRO relies on parameters provided by BGBRO.

1.2 Purpose and objective

The TCBRO is a DOAS-type algorithm for the offline retrieval of vertical column amounts of Bromine Monoxide from measurements by the S-5P/TROPOMI satellite sensor. The algorithms for the TROPOMI raw data treatment (L0 – L1b) and the actual L2 data processing are each described in an algorithm theoretical basis document (ATBD, [AD04]). This Product Format Specification (PFS) document describes the detailed structure and the contained data and metadata of the L2 data files produced by TCBRO.

Slightly deviating from the file format of the current operational S-5P algorithms, the TCBRO L2 format follows the guidelines for a somewhat simplified format, as proposed by S5P-PAL and ESA and described in [AD02].

1.3 Document overview

Chapter 2 lists applicable and reference documentation relevant to this product. Chapter 3 gives an overview of terms, definitions and abbreviations. Chapter 4 describes the TCBRO L2 product and summarizes validation activities. Chapter 5 lists the current structure of S5P/TROPOMI L2 files. Metadata and attributes are described in chapter 6. All elements common to all S5P/TROPOMI L2 products are mentioned in chapter 7. The content of the TCBRO BrO L2 files is given in chapter 8.

2 Applicable and reference documents

2.1 Applicable documents

- [AD01] Tailoring of the Earth Observation File Format Standard for the Sentinel 5-Precursor Ground Segment; source: ESA; ref: S5P-TN-ESA-GS-106; issue: 2.2; date: 2015-02-20.
- [AD02] S5P-PAL: Sentinel 5P Product Algorithm Laboratory – L2 Processor File Format Guidelines; source: S&T; ref: ST-ESA-S5P_PAL-L2FFG-001; issue: 1.3; date: 2022-03-14.
- [AD03] Terms, and symbols in the TROPOMI Algorithm Team; source: KNMI; ref: SN-TROPOMI-KNMI-L2-049-MA; issue: 1.0.0; date: 2015-07-16.
- [AD04] S5P/TROPOMI Total BrO Algorithm TCBRO – Algorithm Theoretical Baseline Document, source: BIRA-IASB; ref: S5P- BIRA-L2-TCBRO- ATBD; issue: 1.1.0; date: 2022-06-17.

2.2 Reference documents

- [RD01] Sentinel-5p + Innovation -Theme 1: CHOCHO, Algorithm Theoretical Baseline Document, source: BIRA-IASB, ref: S5p+I_CHOCHO_BIRA_ATBD; issue: 2.1; date: 2020-11-16.
- [RD02] S5P/TROPOMI ATBD of the formaldehyde tropospheric column product, source: BIRA-IASB; ref: S5P- BIRA-L2-400F- ATBD; issue: 2.2.0; date: 2020-06-15.

2.3 Electronic references

- [URL01] <https://atmospherictoolbox.org/qdoas/>
- [URL02] https://uv-vis.aeronomie.be/software/QDOAS/QDOAS_manual.pdf

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are used in the development program for the TROPOMI L2 data processors are described in [AD03]. Terms, definitions and abbreviated terms that are specific for this document can be found below.

3.1 Acronyms and abbreviations

AMF	Air Mass Factor
BGBRO	BackGround correction auxiliary algorithm for TCBRO
BrO	Bromine Monoxide
DOAS	Differential Optical Absorption Spectroscopy
NetCDF	Network Common Data Form
SCD	Slant Column Density
TCBRO	Total Column BrO retrieval algorithm
TROPOMI	Tropospheric Monitoring Instrument
VCD	Vertical Column Density

4 TCBRO L2 format description.

4.1 TCBRO processor

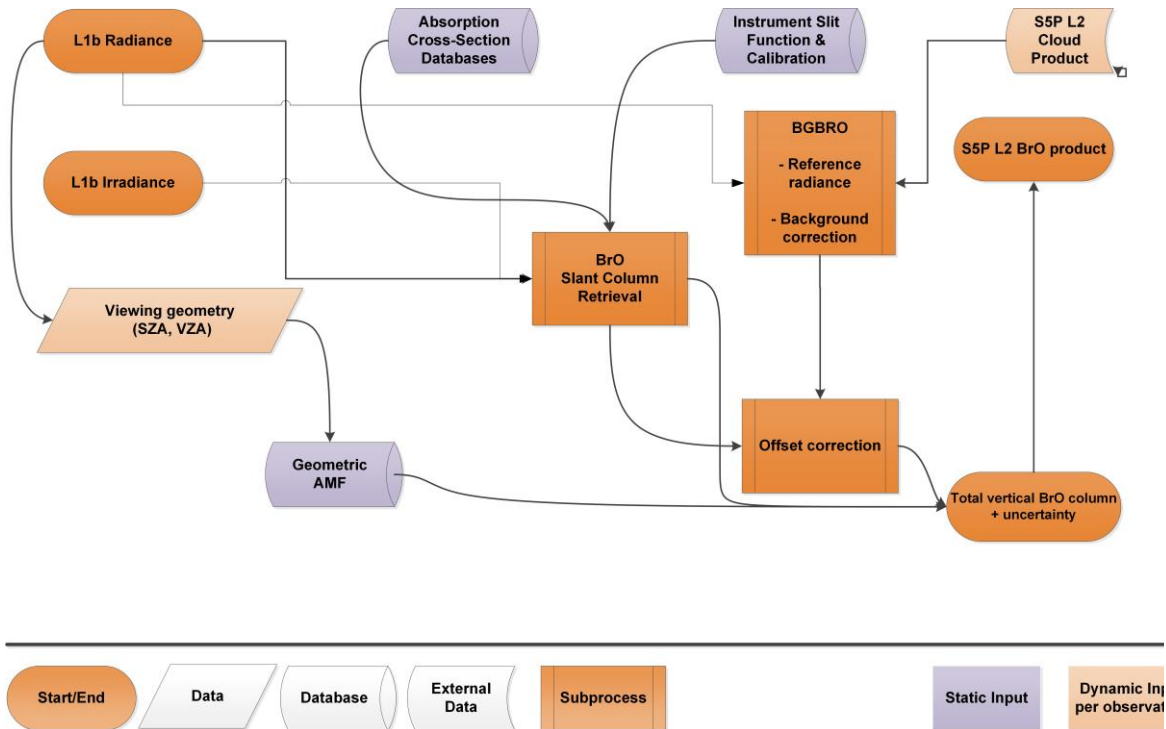


Figure 1: High-level overview of the TCBRO processor algorithm

Figure 1 gives an overview of the algorithm workflow, input and output. The resulting S5P L2 BrO product files are the subject of this document. A detailed description of the algorithm can be found in [RD01].

The total bromine monoxide total vertical column retrieval from S5P data follows a classic DOAS scheme: first, a slant column density (SCD) is derived from the L1b spectra by the DOAS fitting procedure. Like with all minor trace gases, like for example formaldehyde [RD02] and glyoxal [RD01], systematic offsets occur in the derived SCD's. Those are corrected for by means of the background parameters derived by the auxiliary processor BGBRO. As a final step, the corrected slant columns are converted into a vertical column density (VCD) by means of an air mass factor (AMF). In its current shape, TCBRO applies a geometric AMF, depending only on the solar and observation zenith angles. For most scenes this is considered sufficient to obtain a reliable BrO total VCD.

4.2 Product Format Specification

The current TCBRO L2 files are stored as netCDF-4 files and structured according to the guidelines provided in [AD02]. This document outlines a somewhat simpler internal file organization than used for the current operationally produced S5P L2 products, but provides an equivalent structure.

4.2.1 File generation

The TCBRO algorithm generates one L2 file for each L1b orbit file. The BGBRO background processor generates 2 files per day of measurement: one that provides the reference radiance spectrum and one that provides all parameters required for TCBRO to perform the SCD offset correction.

4.2.2 File name specification.

Files generated by S5P L1b>L2 and auxiliary processor are required to fulfill certain file name regulations. Those are outlined in [AD02]. Following these rules, the files generated by TCBRO and BGBRO are named as outlined in Table 1.

Table 1. File naming format for the TCBRO and BGBRO output files.

Processor: TCBRO	Frequency: One file for every orbit
File name format: S5P_{ffff}_L2__TCBRO__{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{ooooo}_{cc}_{pppppp}_{YYYYMMDDThhmmss}.nc	
Processor: BGBRO	Frequency: One file per day per day of measurements
File name format: S5P_{ffff}_AUX_RARBD3_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}.nc	
Processor: BGBRO	Frequency: One file per day per day of measurements
File name format: S5P_{ffff}_AUX_BGBRO__{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}.nc	

The date/time sub-strings in each file name represent respectively: the start of the first measurement in the file, the start of the last measurement in the file, and the start of file creation. The ffff field is the product file class and is dynamically set to 'PAL_' if the file is generated on the S5P-PAL system or to 'OFFL' otherwise.

5 TCBRO L2 file format specification

The sections below outline the file structure and content of the TCBRO L2 output files.

The file structure follows the guidelines as outlined in [AD02], therewith providing a simpler file structure than those of L2 files of current operational products.

5.1 Global attributes

Name	Value	Description
Conventions	"CF-1.7"	CF (Climate and Forecast) conventions used for this product.
Institution	"BIRA-IASB"	Institution responsible for the processing.
source	"Sentinel 5 precursor, TROPOMI, space-borne remote sensing, L2"	Fixed value.
history	"{YYYY-MM-DDThh:mm:ssZ} {executable} {arguments}"	Time of file creation in format "YYYY-MM-DDThh:mm:ssZ" and processor execution.
summary	"TROPOMI/S5P BrO L2 Swath 5.5x3.5km"	Fixed for this product.
id	S5P_{ffff}_L2_TCBRO_{YYYYMMDDThmmss}_{YYYYMMDDThmmss}_{oooo}_{cc}_{ppppp}_{YYYYMMDDThmmss}	File id containing file class and measurement start, stop, and file creation date/time. See also Table 1 and [AD02].
time_reference	"{YYYY-MM-DDThh:mm:ssZ}"	Start of the day of sensing time.
collection_identifier	"{xx}"	Two character collection number. Same as is included in the filename. Example: "01"

time_coverage_start	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of first measurement, to millisecond precision.
time_coverage_end	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of last measurement, to millisecond precision.
Time_coverage_resolution	"PT{duration}S"	Duration of scanline in seconds
orbit	nnnnn	Orbit number
processor name	"TCBRO"	Name of the processor
processor_version	"{xx.yy.zz}"	Processor version
processing_center	"{Processing_Station}"	Name of institution where the processing has taken place.
file_class	"OFFL" or "PAL_"	Indicates offline product
footprint	"{GeoJson string}"	Footprint of orbit as GeoJson string
input_files	["aa.ea", "bb.eb", ...]	List of strings containing all input files to the processor

5.2 Group structure

The L2 file contains one top-level group, called PRODUCT, and several subgroups. The group structure is outlined below.

Group name	Depth	Description
PRODUCT	0	Contains the main output variables and dimensions.
SUPPORT_DATA	1	Contains only sub groups.
DETAILED_RESULTS	2	Sub group of SUPPORT_DATA. Contains additional outputs, such as slant columns of all fitted species.

WAVELENGTH_CALIBRATION	3	Subgroup of DETAILED_RESULTS. Contains parameters related to the wavelength calibration procedure performed during the slant column fitting.
GEOLOCATIONS	2	Sub group of SUPPORT_DATA. Lists all parameters related to observation geometry and geo-location.
INPUT_DATA	2	Sub group of SUPPORT_DATA. Contains all parameters that the TCBRO algorithm needs as input.
BACKGROUND_CORRECTION	3	Sub group of INPUT_DATA. Lists parameters generated by the BGBRO auxiliary processor and ingested by TCBRO for background correction purposes.

5.3 The PRODUCT group

The PRODUCT group is the top-level group and contains the main output variables and dimensions. The content of this group is specified below.

Variables in group /PRODUCT:

Variable	Dimensions	Unit	Description
Type	Attribute type	Attribute value	
brominemonoxide_total_vertical_column			
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	BrO total vertical column density.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"vertical column of formaldehyde"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_molecules_per_cm2	NC_FLOAT	6.02214E19	
standard_name	NC_CHAR	"atmosphere mole content of bromine dioxide"	
units	NC_CHAR	"mol m-2"	
brominemonoxide_total_vertical_column_precision			
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	BrO total vertical column density random uncertainty
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"random error of vertical column density"	

multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_molecules_per_cm2	NC_FLOAT	6.02214E19	
standard_name	NC_CHAR	"atmosphere_mole_content_of bromine monoxide standard_error"	
units	NC_CHAR	"mol m-2"	
delta_time			
NC_INT	(time, scanline)	milliseconds	Offset from reference start time of measurement
long_name	NC_CHAR	"offset from reference start time of measurement"	
units	NC_CHAR	"milliseconds since {YYYY-MM-DD 00:00:00}"	
latitude			
NC_FLOAT	(time, scanline, ground_pixel)	degree	Center latitude of ground pixel
bounds	NC_FLOAT	"/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/latitude_bounds"	
long_name	NC_CHAR	"pixel center latitude"	
standard_name	NC_CHAR	"latitude"	
units	NC_CHAR	"degrees_north"	
valid_min	NC_FLOAT	-90.	
valid_max	NC_FLOAT	90.	
longitude			
NC_FLOAT	(time, scanline, ground_pixel)	degree	Center longitude of ground pixel
bounds	NC_FLOAT	"/PRODUCT/SUPPORT_DATA/GEOLOCATIONS/longitude_bounds"	
long_name	NC_CHAR	"pixel center longitude"	
standard_name	NC_CHAR	"longitude"	
units	NC_CHAR	"degrees_east"	
valid_min	NC_FLOAT	-180.	
valid_max	NC_FLOAT	180.	

qa_value			
NC_UBYTE	(time, scanline, ground_pixel)		Quality
add_offset	NC_FLOAT	0.	
comment	NC_CHAR	"A continuous quality descriptor, varying between 0 (no data) and 1 (full quality data). Recommend to ignore data with qa_value < 0.5"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"data quality value"	
scale_factor	NC_FLOAT	0.01	
units	NC_CHAR	"1"	
valid_max	NC_UBYTE	0	
valid_min	NC_UBUTE	100	

Dimension variables in group /PRODUCT:

Name			
Type	Size	Unit	Description
Attribute name	Attribute type	Attribute value	
corner			
NC_FLOAT	(4)	1	Pixel corner dimension
comment	NC_CHAR	"This coordinate variable defines the indices for the pixel corners; index starts a 0 (counter-clockwise, starting from south-western corner of the pixel in ascending part of the orbit)."	
long_name	NC_CHAR	"pixel corner index"	
units	NC_CHAR	"1"	
ground_pixel			
NC_INT	(450)		Across-track pixel index dimension
axis	NC_CHAR	"X"	
comment	NC_CHAR	"This coordinate variable defines the indices across track, from west to east; index starts at 0"	
long_name	NC_CHAR	"across-track dimension index"	
units	NC_CHAR	"1"	
scanline			

NC_INT	{{# scan lines}}		Along-track pixel index dimension
axis	NC_CHAR	"Y"	
comment	NC_CHAR	"This coordinate variable defines the indices along track; index starts at 0"	
long_name	NC_CHAR	"along-track dimension index"	
units	NC_CHAR	"1"	
time			
NC_INT	(1)		Reference time dimension
axis	NC_CHAR	"T"	
comment	NC_CHAR	"The time in this variable corresponds to the time in the time_reference global attribute"	
long_name	NC_CHAR	"reference time for the measurements"	
standard_name	NC_CHAR	"time"	
units	NC_CHAR	"seconds since 2010-01-01 00:00:00"	

5.4 The SUPPORT_DATA group

This is a subgroup of PRODUCT. It has its own sub groups and contains no other elements than those.

5.5 The DETAILED_RESULTS group

Full path to this group: /PRODUCT/SUPPORT_DATA/DETAILED_RESULTS.

In addition to the main output from the TCBRO processor (the BrO total vertical column density), additional parameters are retrieved along with or are available for diagnostic or statistical purposes. Those are stored in the DETAILED_RESULTS group. The group contains one sub group: WAVELENGTH_CALIBRATION, where all diagnostic parameters regarding the wavelength calibration procedure are stored.

Variables in the group DETAILED_RESULTS:

Name	Type	Size	Unit	Description
Attribute name	Attribute type	Attribute value		
brominemonoxide_geometric_air_mass_factor				
NC_FLOAT	(time, ground_pixel)	scanline,		
coordinates	NC_CHAR		"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR		"geometric mass factor"	

units	NC_CHAR		"1"	
brominemonoxide_slant_column_corrected				
NC_FLOAT	(time, scanline, ground_pixel)		mole m ⁻²	The BrO slant column after offset correction.
coordinates	NC_CHAR		"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR		"corrected slant column density"	
multiplication_factor_to_convert_to_DU	NC_FLOAT		2241.15	
multiplication_factor_to_convert_to_per_cm2	NC_FLOAT		6.02214E19	
units	NC_CHAR		"mol m-2"	
brominemonoxide_slant_column_corrected_trueness				
NC_FLOAT	(time, scanline, ground_pixel)		mole m ⁻²	The systematic error on the corrected BrO slant column.
coordinates	NC_CHAR		"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR		"systematic error of the slant column density"	
multiplication_factor_to_convert_to_DU	NC_FLOAT		2241.15	
multiplication_factor_to_convert_to_per_cm2	NC_FLOAT		6.02214E19	
units	NC_CHAR		"mol m-2"	
brominemonoxide_slant_column_correction_flag				
UBYTE	(time, scanline, ground_pixel)		1	
coordinates	NC_CHAR		"/PRODUCT/longitude /PRODUCT/latitude"	
flag_meanings	NC_CHAR		"not-corrected, corrected"	
flag_values	NC_UBYTE		[0,1]	
long_name	NC_CHAR		"slant column density background correction flag"	
units	NC_CHAR		"1"	
brominemonoxide_total_vertical_column_correction				
NC_FLOAT	(time, scanline, ground_pixel)		mole m ⁻²	Correction value on the BrO vertical column.
coordinates	NC_CHAR		"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR		"background correction value which is added to the vertical column density"	
multiplication_factor_to_convert_to_DU	NC_FLOAT		2241.15	

multiplication_factor_to_convert_to_perkm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
brominemonoxide_total_vertical_column_trueness			
NC_FLOAT	(time, scanline, ground_pixel)	mole m ⁻²	The systematic error on the BrO vertical column.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"systematic error of vertical column density"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_perkm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
fitted_radiance_shift			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"radiance wavelength shift from the doas fit"	
units	NC_CHAR	"1"	
fitted_radiance_squeeze			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"radiance wavelength squeeze/stretch from the doas fit"	
units	NC_CHAR	"1"	
fitted_root_mean_square			
NC_FLOAT	(time, scanline, ground_pixel)	1	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"root mean square from the doas fit"	
units	NC_CHAR	"1"	
fitted_slant_columns			
NC_FLOAT	(time, scanline, ground_pixel, number_of_slant_columns)	mol m-2	The retrieved slant column values for all absorbing species.

coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
index_meaning	NC_CHAR	{list of static absorption cross-section input files}	
long_name	NC_CHAR	"slant columns of all absorbers"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_perkm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
fitted_slant_columns_precision			
NC_FLOAT	(time, scanline, ground_pixel, number_of_slant_columns)	mol m-2	Random error on the retrieved slant column values for all absorbing species.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
index_meaning	NC_CHAR	{list of static absorption cross-section input files}	
long_name	NC_CHAR	"slant columns errors of all absorbers"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_perkm2	NC_FLOAT	6.02214E19	
long_name			
units	NC_CHAR	"mol m-2"	
number_of_slant_columns			
NC_INT	(8)		Dimension variable containing the retrieved slant column indices.
long_name	NC_CHAR	"number_of_slant_columns dimension index"	
units	NC_CHAR	"1"	
number_of_spectral_points_in_retrieval			
NC_INT	(time, scanline, ground_pixel)	1	Number of spectral points used in the DOAS retrieval
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Number of spectral points used in the DOAS retrieval"	
units	NC_CHAR	"1"	

Variables in the group DETAILED_RESULTS/WAVELENGTH_CALIBRATION:

Name			
Type	Size	Unit	Description
Attribute name	Attribute type	Attribute value	
calibration_polynomial_coefficients			
NC_FLOAT	(ground_pixel, degrees_of_polynomial_shift)	1	Computed coefficients of the DOAS polynomial function.
long_name	NC_CHAR	"computed coefficients of the polynomial function"	
units	NC_CHAR	"1"	
calibration_subwindows_root_mean_square			
NC_FLOAT	(ground_pixel, number_of_subwindows)	1	
long_name	NC_CHAR	"calibration rms per subwindow"	
units	NC_CHAR	"1"	
calibration_subwindows_shift			
NC_FLOAT	(ground_pixel, number_of_subwindows)	1	
long_name	NC_CHAR	"irradiance wavelengths shift fitted values per subwindow"	
units	NC_CHAR	"1"	
calibration_subwindows_squeeze			
NC_FLOAT	(ground_pixel, number_of_subwindows)	1	
long_name	NC_CHAR	"irradiance wavelengths squeeze fitted values per subwindow"	
units	NC_CHAR	"1"	
calibration_subwindows_wavelength			
NC_FLOAT	(number_of_subwindows)	nm	
long_name	NC_CHAR	"calibration wavelength center in each subwindow"	
units	NC_CHAR	"nm"	

degrees_of_polynomial_shift			
NC_INT	(degrees_of_polynomial_shift)	1	Dimension with polynomial degree indices.
long_name	NC_CHAR	"degrees_of_polynomial_shift dimension index"	
units	NC_CHAR	"1"	
number_of_calibrations			
NC_INT	(ground_pixel)	1	Dimension array with number of calibration indices (one per detector row).
long_name		"number_of_calibrations dimension index"	
units		"1"	
number_of_subwindows			
NC_INT	(#{sub-windows})		Dimension variable containing the sub-window indices.
long_name	NC_CHAR	"number_of_subwindows dimension index"	
units	NC_CHAR	"1"	

5.6 The GEOLOCATIONS group

The full path to this group is /PRODUCT/SUPPORT_DATA/GEOLOCATIONS/.

Variable			
Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value	
geolocation_flags			
NC_UBYTE	(time, ground_pixel)	scanline, 1	Ground pixel quality flag
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
flag_masks	NC_UBYTE	0, 1, 2, 4, 8, 16, 128	
flag_meanings	NC_CHAR	no_error solar_eclipse sun_glint_possible descending night geo_boundary_crossing geolocation_error	
flag_values	NC_UBYTE	0, 1, 2, 4, 8, 16, 128	
long_name	NC_CHAR	"ground pixel quality flag"	
max_val	NC_UBYTE	128	
min_val	NC_UBYTE	0	
units	NC_CHAR	"1"	

latitude_bounds			
NC_FLOAT	(time, scanline, ground_pixel, 4)	degree	Ground pixel corner coordinate latitudes
units	NC_CHAR	"degree north"	
longitude_bounds			
NC_DOUBLE	(time, scanline, ground_pixel, 4)	degree	Ground pixel corner coordinate longitudes
units	NC_CHAR	"degree east"	
satellite_altitude			
NC_FLOAT	(time, scanline)	degree	Satellite altitude
comment	NC_CHAR	"The altitude of the satellite with respect to the geodetic sub satellite point on the WGS84 reference ellipsoid"	
long_name	NC_CHAR	"satellite altitude"	
units	NC_CHAR	"m"	
valid_max	NC_FLOAT	90000.	
valid_min	NC_FLOAT	70000.	
satellite_latitude			
NC_FLOAT	(time, scanline)	degree	Satellite latitude
comment	NC_CHAR	"Latitude of the geodetic sub satellite point on the WGS84 reference ellipsoid"	
long_name	NC_CHAR	"Sub satellite latitude"	
units	NC_CHAR	"degree north"	
valid_max	NC_FLOAT	90.	
valid_min	NC_FLOAT	-90.	
satellite_longitude			
NC_FLOAT	(time, scanline)	degree	Satellite longitude
comment	NC_CHAR	"Longitude of the geodetic sub satellite point on the WGS84 reference ellipsoid"	
long_name	NC_CHAR	"Sub satellite longitude"	
units	NC_CHAR	"degree east"	
valid_max	NC_FLOAT	90.	
valid_min	NC_FLOAT	-90.	
satellite_orbit_phase			
NC_FLOAT	(time, scanline)	1	Satellite fractional orbit phase

comment	NC_CHAR	"Relative offset [0.0, ..., 1.0] of the measurement in the orbit"	
long_name	NC_CHAR	"fractional satellite orbit phase"	
units	NC_CHAR	"1"	
valid_max	NC_FLOAT	1.02	
valid_min	NC_FLOAT	-1.02	
solar_azimuth_angle			
NC_DOUBLE	(time, scanline, ground_pixel)	degree	Solar azimuth angle
comments	NC_CHAR	"Solar azimuth angle at the ground pixel location on the reference ellipsoid. Angle is measured clockwise from the North (East = 90, South = 180, West = -180) "	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"solar azimuth angle"	
standard_name	NC_CHAR	"solar_azimuth_angle"	
units	NC_CHAR	"1"	
valid_max	NC_DOUBLE	180.	
valid_min	NC_DOUBLE	-180.	
solar_zenith_angle			
NC_DOUBLE	(time, scanline, ground_pixel)	degree	Solar zenith angle
comments	NC_CHAR	"Solar zenith angle at the ground pixel location on the reference ellipsoid. Angle is measured away from the vertical"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"solar zenith angle"	
standard_name	NC_CHAR	"solar_zenith_angle"	
units	NC_CHAR	"1"	
valid_max	NC_DOUBLE	180.	
valid_min	NC_DOUBLE	0.	
viewing_azimuth_angle			
NC_DOUBLE	(Time, scanline, ground_pixel)	degree	Viewing azimuth angle
comments	NC_CHAR	"Satellite azimuth angle at the ground pixel location on the reference ellipsoid. Angle is measured clockwise from the North (East = 90, South = 180, West = -180)"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"viewing azimuth angle"	

standard_name	NC_CHAR	"viewing_azimuth_angle"	
units	NC_CHAR	"1"	
valid_max	NC_DOUBLE	180.	
valid_min	NC_DOUBLE	-180.	
viewing_zenith_angle			
NC_DOUBLE	(Time, scanline, ground_pixel)	degree	Viewing zenith angle
comments	NC_CHAR	"Zenith angle of the satellite at the ground pixel location on the reference ellipsoid. Angle is measured away from the vertical"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"viewing zenith angle"	
standard_name	NC_CHAR	"viewing_zenith_angle"	
units	NC_CHAR	"1"	
valid_max	NC_DOUBLE	180.	
valid_min	NC_DOUBLE	0.	

5.7 The INPUT_DATA group

This group contains the parameters that serve as input to the TCBRO processor. This group also contains one sub group: BACKGROUND_CORRECTION, that contains all quantities that are required for the slant column background correction procedure.

The majority of variables in INPUT_DATA are inherited directly from the S5P L2 CLOUD product. Variables marked with an asterisk (*) were introduced in later versions of the CLOUD product and their presence in the TCBRO L2 files therefore depend on the version of the used input L2 CLOUD product file.

The full path of this group is /PRODUCT/SUPPORT_DATA/INPUT_DATA/.

5.7.1 Variables in INPUT_DATA

Variable	Dimensions	Unit	Description
Type	Attribute name	Attribute type	Attribute value
cloud_albedo_crb			
NC_FLOAT	(time, scanline, ground_pixel)	1	Cloud top albedo for a cloud acting as a reflecting boundary (crb).
comment	NC_CHAR	"Albedo of cloud using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Cloud albedo from the CRB model"	

source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"cloud_albedo"	
units	NC_CHAR	"1"	
cloud_albedo_crb_precision			
NC_FLOAT	(time, scanline, ground_pixel)	1	Precision on the cloud top albedo for a cloud acting as a reflecting boundary (crb).
comment	NC_CHAR	"Error of the albedo of cloud using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Cloud albedo precision from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"cloud_albedo_standard_error"	
units	NC_CHAR	"1"	
cloud_fraction_crb			
NC_FLOAT	(time, scanline, ground_pixel)	1	Effective radiometric cloud fraction.
comment	NC_CHAR	"Retrieved effective radiometric cloud fraction using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Effective radiometric cloud fraction from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units	NC_CHAR	"1"	
cloud_fraction_crb_precision			
NC_FLOAT	(time, scanline, ground_pixel)	1	Precision of the effective radiometric cloud fraction.
comment	NC_CHAR	"Error of the retrieved effective radiometric cloud fraction using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"Effective radiometric cloud fraction precision from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units	NC_CHAR	"1"	
cloud_height_crb			

NC_FLOAT	(time, scanline, ground_pixel)	meter	Cloud height considering the cloud as a reflective boundary (crb).
comment	NC_CHAR	"Retrieved height at the level of cloud w.r.t. the geoid/MSL using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"cloud radiometric optical centroid height from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units	NC_CHAR	"m"	
cloud_height_crb_precision			
NC_FLOAT	(time, scanline, ground_pixel)	meter	Precision on the crb cloud height.
comment	NC_CHAR	"Error of retrieved height at the level of cloud w.r.t. the geoid/MSL using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"cloud radiometric optical centroid height precision from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units	NC_CHAR	"m"	
cloud_pressure_crb			
NC_FLOAT	(time, scanline, ground_pixel)	Pascal	Atmospheric pressure at the level of the cloud.
comment	NC_CHAR	"Retrieved atmospheric pressure at the level of cloud w.r.t. the geoid/MSL using the OCRA/ROCINN CRB model"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"cloud radiometric optical centroid pressure from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units	NC_CHAR	"Pa"	
cloud_pressure_crb_precision			
NC_FLOAT	(time, scanline, ground_pixel)	Pascal	Precision on the cloud pressure.
comment	NC_CHAR	"Error of the retrieved atmospheric pressure at the level of cloud w.r.t. the geoid/MSL using the OCRA/ROCINN CRB model"	

coordinates	NC_CHARNC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"cloud radiometric optical centroid pressure precision from the CRB model"	
source	NC_CHAR	"crb"	
standard_name	NC_CHAR	"TBD"	
units		"Pa"	
eastward_wind*			
NC_FLOAT	(time, scanline, ground_pixel)	meters per second	Eastward wind from ECMWF at 10 meter height level.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	Eastward wind from ECMWF at 10 meter height level	
standard_name	NC_CHAR	eastward_wind	
units	NC_CHAR	"m s-1"	
instrument_configuration_identifier			
NC_INT	(time, scanline)	1	Each combination of instrument settings is referred to as an instrument configuration and is identified by an instrument configuration ID, a number in the range [1;65535].
comment	NC_CHAR	"The Instrument Configuration ID defines the type of measurement and its purpose. The number of instrument configuration IDs will increase over the mission as new types of measurements are created and used"	
long_name	NC_CHAR	"IcID"	
instrument_configuration_version			
NC_SHORT	(time, scanline)	1	Each instrument configuration may be altered during the instrument lifetime. The configuration version can be found here.
comment	NC_CHAR	"version of the instrument_configuration_identifier"	
long_name	NC_CHAR	"IcVersion"	
northward_wind*			
NC_FLOAT	(time, scanline, ground_pixel)	meters per second	Northward wind from ECMWF at 10 meter height level.

coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long name	NC_CHAR	Northward wind from ECMWF at 10 meter height level	
standard_name	NC_CHAR	northward_wind	
units	NC_CHAR	"m s-1"	
sea_ice_cover*			
NC_FLOAT	(time, scanline, ground_pixel)	1	Sea-ice cover fraction.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"sea-ice-cover"	
source	NC_CHAR	"ECMWF"	
units	NC_CHAR	"1"	
snow_cover*			
NC_FLOAT	(time, scanline, ground_pixel)	1	Snow cover fraction.
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"snow-cover"	
source	NC_CHAR	"ECMWF"	
units	NC_CHAR	"1"	
snow_ice_flag			
NC_UBYTE	(time, scanline, ground_pixel)	1	Flag indicating the presence of snow or ice at the ground pixel center.
comment	NC_CHAR	"flag indicating snow/ice at the center of ground pixel"	
coordinates		"/PRODUCT/longitude /PRODUCT/latitude"	
flag_meaning	NC_CHAR	"snow-free_land snow_ice"	
flag_values	NC_UBYTE	0, 1	
long_name	NC_CHAR	"snow-ice mask"	
source	NC_CHAR	"NSIDC/NISE"	
threshold	NC_CHAR	"0.3"	
units	NC_CHAR	"1"	
snow_ice_flag_nise			
NC_UBYTE	(time, scanline, ground_pixel)	1	Flag indicating the presence of snow or ice at the ground pixel center.
comment	NC_CHAR	"flag indicating snow/ice at the center of ground pixel"	
coordinates		"/PRODUCT/longitude /PRODUCT/latitude"	

flag_meaning	NC_CHAR	"snow-free_land sea_ice_1_percent ... sea_ice_100_percent permanent_ice snow mixed_pixels_at_coastlines suspect_ice_value corners ocean"	
flag_values	NC_UBYTE	0, 1, ..., 100, 101, 103, 252, 253, 254, 255	
long_name	NC_CHAR	"snow-ice mask"	
source	NC_CHAR	"NSIDC/NISE"	
units	NC_CHAR	"1"	
surface_altitude			
NC_FLOAT	(time, scanline, ground_pixel)	meter	Mean surface altitude derive from sub-pixel values.
comment	NC_CHAR	"The mean of the sub-pixels of the surface altitude"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"surface altitude"	
source	NC_CHAR	"http://topotools.cr.usgs.gov/gmted_viewer/"	
standard_name	NC_CHAR	"surface_altitude"	
units	NC_CHAR	"m"	
surface_altitude_precision			
NC_FLOAT	(time, scanline, ground_pixel)	meter	The standard-deviation of sub-pixels used in calculating the mean surface altitude derive from sub-pixel values.
comment	NC_CHAR	The standard-deviation of sub-pixels used in calculating the mean surface altitude derive from sub-pixel values.	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	
long_name	NC_CHAR	"surface altitude precision"	
source	NC_CHAR	"http://topotools.cr.usgs.gov/gmted_viewer/"	
standard_error_multiplier	NC_FLOAT	1.0	
standard_name	NC_CHAR	"surface_altitude standard error"	
units	NC_CHAR	"m"	
surface_classification			
NC_UBYTE	(time, scanline, ground_pixel)		Classification of the surface type (land, water, etc.) of the ground pixel.
Comment	NC_CHAR	"flag indicating land/water and futher surface classification for the ground pixel"	
coordinates	NC_CHAR	"/PRODUCT/longitude /PRODUCT/latitude"	

flag_masks	NC_UBYTE	3, 3, 3, 3, 4, 249, 249, ..., 249	
flag_meanings	NC_CHAR	<p>“land water some_water coast value_covers_majority_of_pixel water+shallow_ocean, water+shallow_inland_water, water+ocean_coastline- lake_shoreline, water+intermittent_water, water+deep_inland_water, water+continental_shelf_ocean, water+deep_ocean, land+urban_and_built-up_land, land+dryland_cropland_and_pasture, land+irrigated_cropland_and_pasture, land+mixed_dryland-irrigated_cropland_and_pasture, land+cropland-grassland_mosaic, land+cropland- woodland_mosaic, land+grassland, land+shrubland, land+mixed_shrubland-grassland, land+savanna, land+deciduous_broadleaf_forest, land+deciduous_needleleaf_forest, land+evergreen_broadleaf_forest, land+evergreen_needleleaf_forest, land+mixed_forest, land+herbaceous_wetland, land+wooded_wetland, land+barren_or_sparsely_vegetated, land+herbaceous_tundra, land+wooded_tundra, land+mixed_tundra, land+bare_ground_tundra, land+snow_or_ice”_</p>	
flag_values	NC_UBYTE	0, 1, 2, 3, 4, 9, 17, 25, 33, 41, 49, 57, 8, 16, 24, 32, 40, 48, 56, 64, 72, 80, 88, 96, 1, 4, 112, 120, 128, 136, 144, 152, 160, 168, 176, 184	
long_name	NC_CHAR	“land-water mask”	
source	NC_CHAR	<p>“USGS (http://edc2.usgs.gov/glcc/globdoc2_0.php) and NASA SDP toolkit (http://newsroom.gsfc.nasa.gov/sdptoolkit/toolkit.html) ”</p>	
units	NC_CHAR	“1”	
surface_pressure			
NC_FLOAT	(time, scanline, ground_pixel)	Pascal	Surface air pressure.
Coordinates	NC_CHAR	“/PRODUCT/longitude /PRODUCT/latitude”	
long_name	NC_CHAR	“surface_air_pressure”	
source	NC_CHAR	“”	
standard_name	NC_CHAR	“surface_air_pressure”	
units	NC_CHAR	“Pa”	
surface_temperature*			
NC_FLOAT	(time, scanline, ground_pixel)	Kelvin	Surface air temperature.
coordinates	NC_CHAR	“/PRODUCT/longitude /PRODUCT/latitude”	
long_name	NC_CHAR	“surface_air_temperature”	
source	NC_CHAR	“”	

standard_name	NC_CHAR	"surface_air_temperature"
units	NC_CHAR	"K"

5.7.2 The INPUT_DATA/BACKGROUND_CORRECTION group

Attribute	Attribute type	Attribute value	Description
reference_radiance_time_range	NC_CHAR	"{YYYYMMDDThhmmss_YYYYMMDDThhmmss}"	Time interval (start_end) of the measurements used to determine the radiance reference spectra.
background_scd_time_range	NC_CHAR	"{YYYYMMDDThhmmss_YYYYMMDDThhmmss}"	Time interval (start_end) of the measurements used to derive the slant column values over the reference region..

5.7.3 Variables in INPUT_DATA/BACKGROUND_CORRECTION

Variable			
Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value	
amf_scd0_average			
NC_FLOAT	(ground_pixel)	1	Per-row average geometric amf over the reference sector.
units	NC_CHAR	"1"	
earthshine_reference_radiance			
NC_FLOAT	(ground_pixel, wavelengths)		Radiance reference spectrum per detector row.
units	NC_CHAR	"mol.m-2.nm-1.sr-1.s-1"	
earthshine_reference_wavelength			
NC_FLOAT	(ground_pixel, wavelengths)	nanometer	Radiance reference wavelength grid.
units	NC_CHAR	"nm"	
offsets			
NC_FLOAT	(ground_pixel)	mole m ⁻²	VCD offset .
units	NC_CHAR	"mol m-2"	
offsets_scd0			

NC_FLOAT	(ground_pixel)	mole m ⁻²	SCD offset.
units	NC_CHAR	"mol m-2"	
wavelengths			
NC_INT	({# wavelengths})	nanometer	Wavelength dimension index of the reference spectrum.

6 The BGBRO radiance reference auxiliary file

The core component of the TCBRO algorithm is the QDOAS slant column retrieval tool [URL01]. The generated auxiliary file with radiance reference spectral information is ingested directly by QDOAS and therefore follows a strict format that QDOAS can recognize. The file name is formatted as specified in Table 1. The content of this file is outlined below.

Global attributes:

Name	Value	Description
Conventions	"CF-1.7"	CF (Climate and Forecast) conventions used for this product.
input_files	["aa.ea", "bb.eb", ...]	String list with all input files to the processor.
institution	"BIRA-IASB"	Institution responsible for the processing.
history	"{YYYY-MM-DDThh:mm:ssZ" {executable} {arguments}"	Time of file creation in format "YYYY-MM-DDThh:mm:ssZ"
summary	"Radiance as reference file in APEX format for QDOAS based on daily averaged radiances"	Fixed for this product.
id	"S5P_{ffff}_AUX_BGBRO_{YYYYMMDDThhmmss}_{ YYYYMMDDThhmmss }_{YYYYMMDDThhmmss}"	File id containing file class and measurement start, stop, and file creation date/time.
lat_bound	{lat_min}, {lat_max}	Latitude boundaries of the reference sector.
lon_bound	{lon_min}, {lon_max}	Longitude boundaries of the reference sector.
measurement_date	"DD/MM/YYYY"	The date indicating the S5P measurements date used for generating the content of this file.
time_coverage_start	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of first measurement.
time_coverage_end	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of last measurement.

processor name	"BGBRO"	Name of the processor
processor_version	"{xx.yy.zz}"	Processor version
processing_center	"{Processing Station}"	Institution where the processing has taken place.
file_class	"OFFL" or "PAL_"	Indicates offline product

Copy largely from L2 file

Variables of the root group '/':

Variable			
Type	Dimensions	Unit	Description
Attribute name	Attribute type	Attribute value	
col_dim			
NC_FLOAT	(450)	1	Matrix column dimension, with index representing the S5P detector row.
number_radiances			
NC_SHORT	(col_dim)		Number of radiance values involved in calculating the average radiance for each detector row.
reference_radiance			
NC_DOUBLE	(col_dim, spectral_dim)		The average reference radiance spectrum per detector row.
units	NC_CHAR	"mol.m-2.nm-1.sr-1.s-1"	
reference_wavelength			
NC_DOUBLE	(col_dim, spectral_dim)	nanometer	The wavelength spectrum per detector row.
units	NC_CHAR	"nm"	
spectral_dim			
NC_FLOAT	({# wavelengths})		Spectral dimension. The size depends on the wavelength grid requested by the BGBRO processor

use_row			
NC_BYTE	(450)		Diagnostic parameter. Says for each detector row if a valid radiance was calculated (value = 1) or not (value = 0).
valid_max	NC_BYTE	1	
valid_min	NC_BYTE	0	

7 The BGBRO background correction file

The second type of output file generated by BGBRO contains information relevant to the main processor TCBRO for the offset correction on the derived slant column data. The content of this file is outlined below.

File name format (see also Table 1):

S5P_{ffff}_AUX_BGBRO_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}.nc

The file contains only a single root group.

Global attributes:

Name	Value	Description
Conventions	"CF-1.7"	CF (Climate and Forecast) conventions used for this product.
input_files	["aa.ea", "bb.eb", ...]	String list with all input files to the processor.
institution	"BIRA-IASB"	Institution responsible for the processing.
history	"{YYYY-MM-DDThh:mm:ssZ} {executable} {arguments}"	Time of file creation in format "YYYY-MM-DDThh:mm:ssZ"
summary	"TROPOMI/S5P BrO L2 Background correction parameters"	Fixed for this product.
id	"S5P_{ffff}_AUX_BGBRO_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}_{YYYYMMDDThhmmss}"	File id containing measurement start, stop, and file creation date/time. ffff is either 'PAL_' or 'OFFL'
lat_bound	{lat_min}, {lat_max}	Latitude boundaries of the reference sector.
lon_bound	{lon_min}, {lon_max}	Longitude boundaries of the reference sector.
time_coverage_start	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of first measurement.
time_coverage_end	"{YYYY-MM-DDThh:mm:ss.fffZ}"	Start time of last measurement.

processor name	"BGBRO"	Name of the processor
processor_version	"{xx.yy.zz}"	Processor evrsion
processing_center	"{Processing Station}"	Institution where the processing has taken place.
file_class	"OFFL" or "PAL_"	Indicates offline product generated on S5P_PAL or elsewhere.

Variables in the root group '/':

Variable	Type	Dimensions	Unit	Description	
Attribute name	Attribute type	Attribute value			
count_row					
NC_INT	(ground_pixel)	1		Number of measurements contributing to the reference sector row values.	
comment units	NC_CHAR NC_CHAR	"Number of measurements used in calculating the average SCD over the reference sector"		"1"	
ground_pixel					
NC_INT	(450)	1		Detector row dimension index.	
axis comment long_name units	NC_CHAR NC_CHAR NC_CHAR NC_CHAR	"X"			"This coordinate variable defines the indices across track, from west to east; index starts at 0"
		"across-track dimension index"			"1"
brominemonoxide_slant_column_average_background					
NC_FLOAT	(ground_pixel)	mole cm⁻²		Per-row average SCD over the reference sector	
comment multiplication_factor_to convert_to_DU	NC_CHAR NC_FLOAT	"Average BrO slant column over the reference sector, calculated per row"		2241.15	

multiplication_factor_to_convert_to_molecules_per_cm2	NC_FLOAT	6.02214E19	
units		"mol m-2"	
brominemonoxide_total_vertical_column_background			
NC_FLOAT	(ground_pixel)	mole m ⁻²	Assumed BrO background VCD.
	NC_FLOAT	6.02214E19	
comment	NC_CHAR	"Adopted background vertical column value"	
multiplication_factor_to_convert_to_DU	NC_FLOAT	2241.15	
multiplication_factor_to_convert_to_molecules_per_cm2	NC_FLOAT	6.02214E19	
units	NC_CHAR	"mol m-2"	
brominemonoxide_geometric_air_mass_factor_background			
NC_FLOAT	(ground_pixel)	1	Per-row averaged geometric AMF over the reference sector.
comment	NC_CHAR	"Average AMF per row over the reference sector"	
units	NC_CHAR	"1"	

