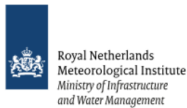




# S5P Mission Performance Centre Carbon Monoxide [L2\_\_CO\_\_\_\_] Readme



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<sup>1</sup> The S5PVT AO project summaries can be found at  
<https://earth.esa.int/eogateway/news/announcement-of-opportunity-for-s5pvt>

## CHANGE LOG

Reason for change	Issue	Revision	Date
<ul style="list-style-type: none"> <li>Table 2: Adapting to version 02.02.00 of the processor.</li> <li>Section 3.2: Validation results shortened, pointing to the routine Validation reports.</li> <li>Section 4.1 &amp; section 0: some text moved from section 4.1 (Known Data Quality Issues) to section 0 (Solved Data Quality Issues).</li> <li>Section 6.1: added format changes related to version 02.02.00.</li> </ul>	2	0	05/07/2021
Table 2: Adapting to version 02.03.01 of the processor	2	1	17/11/2021
<ul style="list-style-type: none"> <li>Table 2: Adapting to version 02.04.00 of the processor.</li> <li>Section 6.1: added format changes related to version 02.02.00.</li> </ul>	2	2	20/07/2022

# 1 Summary

This is the Product Readme File (PRF) for the Copernicus Sentinel 5 Precursor Tropospheric Monitoring Instrument (S5P/TROPOMI) Carbon Monoxide total column level 2 data product and is applicable for the Offline (OFFL) and Near Real Time (NRTI) timeliness data product.

Product Identifier: **L2\_CO**

Example filename for the OFFL and NRTI product:

**S5P\_OFFL\_L2\_CO\_\_\_\_\_20210908T001010\_20210908T015140\_20226\_02\_020200\_20210909T135900.nc**

**S5P\_NRTI\_L2\_CO\_\_\_\_\_20210908T002709\_20210908T003209\_20226\_02\_020200\_20210908T012952.nc**

The file name convention is described in more detail in the Product User Manual (PUM) [RD03]. The OFFL product has the following Digital Object Identifier (DOI): <http://doi.org/10.5270/S5P-bj3nry0> for the NRTI product a corresponding identifier is not applicable.

This Readme file describes the current processing baseline, product and quality limitations, and product availability status. More information on this data product is available from the Copernicus Sentinel product webpage:

<https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>,

and from the TROPOMI product webpage <http://www.tropomi.eu/data-products>.

The data file contains the `carbonmonoxide_total_column`, which gives the total atmospheric column between the surface and the top of atmosphere. The respective random error originating from the spectral fit is given in the `carbonmonoxide_total_column_precision`. As a user guideline for the data quality a `qa_value` is given with the data. To avoid misinterpretation of the data quality, it is recommended at the current stage to only use those pixels with a `qa_value` above 0.5.

The NRTI data stream delivers the CO column data product within 3 hours after sensing, whereas the OFFL data product is available a few days after acquisition. Because of the different timeliness, the NRTI product is given in 5 min data granules whereas the OFFL data product per satellite orbit. Both the OFFL and NRTI processing chains employ the same algorithm. Since processor version 01.03.02, the same configuration settings are used for both data streams and so the data products are expected to be of the same quality. For earlier versions, the NRTI and OFFL data product differ in the way the solar irradiance measurements are used. The NRTI processing requires the L1B reflectance spectra as input to the retrieval, whereas the OFFL processing is based on the Earthshine radiance measurements and uses a spectral deconvolution of the solar irradiance spectra during the algorithm initialization to infer a line-by-line solar spectrum as an input to the retrieval. More details on the two processing streams are given in the product Algorithm Theoretical Basis Document (ATBD) [RD02].

**Note:** Starting from processor version 2.4.0, new improved Level 1b version 2.1 data products are used as input [RD06].

Independent validation by MPC Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that OFFL CO total column data is compliant with the requirements as defined in the **S5P Calibration and Validation Plan** [RD01], see Table 1.

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after September 2021 include validation results based on processor version 2.x.x.

Parameter	Data product	Vertical Resolution	Bias	Random
Total column	Carbon monoxide (CO)	Total column	15%	10%

Table 1: Mission data requirements for the CO product, extracted from [RD01]

## 2 Processing baseline description

Table 2 contains the history of the CO processor versions. Note that the processor version for CO is changing when there is a change to any of the products belonging to the NL-L2 processor suite (NO2, CO, CH4, AI, ALH, O3 PR) even if the change is not affecting the CO product.

Processor Version	In operation from	In operation until	Relevant improvements
02.04.00	OFFL: orbit 24655, 2022-07-17 NRTI: orbit 24697, 2022-07-20	Current Version	<ul style="list-style-type: none"> <li>Total column averaging kernels in unitless representation</li> <li>Null-space filling used for the retrieval parameters</li> <li>The TM5 <i>a priori</i> profiles are included in the output</li> </ul> <p><b>Note:</b> Starting from this processor version, new improved Level 1b version 2.1 data products are used as input [RD06]</p>
02.03.01	OFFL: orbit 21188, 2021-11-14 NRTI: orbit 21223, 2021-11-17	Orbit 24654, 2022-07-17 Orbit 24697, 2022-07-20	No changes with respect to previous version
02.02.00	OFFL: orbit 19258, 2021-07-01 NRTI: orbit 19308, 2021-07-05	Orbit 21187, 2021-11-14 Orbit 21222, 2021-11-17	<ul style="list-style-type: none"> <li>Update CH<sub>4</sub>, CO and H<sub>2</sub>O cross sections in the CO and CH<sub>4</sub> processors: the updated cross sections are based on DLR Scientific Exploitation of Operational Missions – Improved Atmospheric Spectroscopy Databases (SEOM-IAS) spectroscopy (<a href="https://zenodo.org/record/1009126#.YJurduvRaL4">https://zenodo.org/record/1009126#.YJurduvRaL4</a>)</li> <li>Added CO destriping algorithm for OFFL data</li> </ul> <p><b>Note:</b> Starting from this processor version, new improved Level 1b version 2.0 data products are used as input [RD06]</p>
01.04.00	OFFL: orbit 16213, 2020-11-29 NRTI: orbit 16259, 2020-12-02	Orbit 19257, 2021-07-01 Orbit 19306, 2021-07-05	No changes with respect to previous version
01.03.02	OFFL: orbit 8815, 2019-06-26 NRTI: orbit 8906, 2019-07-03	Orbit 16212, 2020-11-29 Orbit 16256, 2020-12-02	OFFL and NRTI processing chains employ the same algorithm since this version
01.03.01	OFFL: orbit 7907, 2019-04-23 NRTI: orbit 8000, 2019-04-30	Orbit 8814, 2019-06-26 Orbit 8906, 2019-07-03	No changes with respect to previous version
01.03.00	OFFL: orbit 7425, 2019-03-20 NRTI: orbit 7519, 2019-03-27	Orbit 7906, 2019-04-23 Orbit 7999, 2019-04-30	Added new variables: <code>eastward_wind</code> and <code>northward_wind</code>

01.02.02	RPRO: orbit 2818, 2018-04-30 OFFL: orbit 5833, 2018-11-28 NRTI: orbit 5932, 2018-12-05	Orbit 3847, 2018-07-11 Orbit 7424, 2019-03-20 Orbit 7518, 2019-03-27	Sun glint was wrongly considered in the qa_value calculation in previous versions
01.02.00	OFFL: orbit 5236, 2018-10-17 NRTI: orbit 5741, 2018-11-22	Orbit 5832, 2018-11-28 Orbit 5929, 2018-12-05	Adjusted qa_value in case of eclipse
01.01.00	OFFL: orbit 3848, 2018-07-11	Orbit 5235, 2018-10-17	Correction of a bug for qa_value and updated definition
01.00.02	OFFL: orbit 3661, 2018-06-28	Orbit 3847, 2018-07-11	Initial operational version

Table 2: History of CO processor versions. In orange, the data versions that are no longer available to the users on the Pre-operations hub.

### 3 Product Quality

#### 3.1 Recommendations for data usage

Both for the OFFL and NRTI product, it is recommended to use TROPOMI CO data associated with a quality assurance value  $qa\_value > 0.5$ . The  $qa\_value$  is provided as part of the CO data product and the definition used in the current data release is summarized in Table 3.

$qa\_value$	Condition	Remark
1.0	$\tau_{aer} < 0.5$ and $z_{cld} < 500$ m	clear-sky and clear-sky like observations
0.7	$\tau_{aer} \geq 0.5$ and $z_{cld} < 5000$ m	mid-levels cloud
0.4	$(\tau_{aer} \geq 0.5$ and $z_{cld} \geq 5000$ m) or $(\tau_{aer} \leq 0.5$ and $z_{cld} \geq 500$ m)	high clouds, experimental data set
0.0	$irow \leq 1$ or $SZA \geq 80^\circ$ or defective product	corrupted or defective data

Table 3:  $qa\_value$  parameter definition

Here,  $irow \leq 1$  filters out the two most westward pixels because of unresolved calibration issues. For low sun with Solar Zenith Angles  $SZA \geq 80^\circ$  the retrieval is most sensitive to radiometric and retrieval errors due to the long light path through the atmosphere. We recommend using only data with a  $qa\_value = 1$  in case the averaging kernel is not applied. Data with a  $qa\_value = 0.7$  are of similar quality provided the averaging kernel is used to account for the vertical retrieval sensitivity in the presence of mid-level clouds. Quality assurance values of  $qa\_value = 0.4$  represent experimental data to be used with caution.

For further details, data users are encouraged to read the Product User Manual (PUM, [RD03]) and Algorithm Theoretical Basis Document (ATBD, [RD02]) associated with this data product, both available on <https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>.

The TROPOMI CO product provides total column averaging kernels for the individual retrievals from each ground pixel of the satellite provided in the variable `column_averaging_kernel`. The total column-averaging kernel is unit less since version 02.04.00, and defined on vertical partial column profiles which is a more common representation. In previous processor versions (<02.04.00) the variable `column_averaging_kernel` had the unit meters and needed to be divided by 1000 m to transfer it to its unit less representation. This is not needed anymore.

The TROPOMI CO retrieval is based on the profile scaling inversion and Borsdorff et al. (2014) [RD05] showed that in this case the equation  $x_{ref} = \mathbf{a} * x_{ref}$  holds which means that the total column averaging kernel  $\mathbf{a}$  cannot smooth the vertical CO reference profile  $x_{ref}$  that is used for scaling within the inversion. This simplifies the validation equation  $x_{ret} = \mathbf{a} * x_{true} + (\mathbf{a} - 1) * x_{ref}$  to  $x_{ret} = \mathbf{a} * x_{true}$ . Hence, this means vertical CO profiles from e.g. model calculations or airborne measurement can be smoothed by the total column averaging kernel  $\mathbf{a}$  and compared to the CO total columns of TROPOMI without the need of the reference profile  $x_{ref}$  that is used within the TROPOMI CO retrieval. The total column-averaging kernel of TROPOMI is defined for vertical altitude layers, hence the values and shape of the kernel depends on this vertical grid. We highly recommend for validation purposes not interpolating the averaging kernel on different vertical grids but integrate the vertical CO profiles used for validation or inter-comparison on the partial column layering used for the TROPOMI CO total column averaging kernel that consists of equidistant 1000m thick layers and starts from the surface altitude provided for each ground pixel of TROPOMI.

## 3.2 Validation results

Independent validation by MPC Cal/Val experts and the Sentinel-5 Precursor Validation Team (S5PVT) concludes that the version 1.x.x of the OFFL CO total column data is in good overall agreement with (i) reference measurements collected from the TCCON and NDACC global ground-based networks, and (ii) the corresponding satellite data products from MOPITT. In particular, a bias of <10% found in the data comparisons is well within the mission requirements (Table 1) of  $\leq 15\%$ . The scatter of the data around this bias also complies with mission requirements of  $\leq 10\%$ . The comparison of S5p TROPOMI and MOPITT CO total columns supports the findings of the data product validation with ground-based measurements. The NRTI product was subject to an additional positive bias of 3-4 % but since processor version 01.03.02, the same configuration settings are used for the NRTI and OFFL data processing streams and therefore the data products are of the same quality.

The quality of the processor version 2.x.x is routinely assessed since the production started in July 2021, and the results is that, as expected, the data are slightly biased low compared to version 1.

Up to date validation results are available in the Routine Operations Consolidated Validation Reports (ROCVR) that are accessible through the MPC Validation Data Analysis Facility (VDAF) website at <http://mpc-vdaf.tropomi.eu>. The ROCVR reports are issued quarterly, and reports released after September 2021 include validation results based on processor version 2.x.x.

**We thank all the TCCON and NDACC PI's for providing the data without which this validation study would not have been possible.**



## 4 Data Quality Remarks

### 4.1 Known Data Quality Issues

Currently, the following data quality issues are known, not covered by the quality flags, and should be kept in mind when looking at the carbon monoxide product and also at preliminary validation results.

#### Stripes

Single TROPOMI overpasses show stripes of erroneous CO values < 10% in the flight direction, probably due to calibration issues of TROPOMI. Borsdorff et al. 2019 [RD04] suggested two methods to correct the high-frequency variations of the CO measurements across flight direction per orbit. The fixed masked destriping method (FFM) is based on median filtering of the detected features in flight direction and the Fourier Filter Destriping (FFD) that corrects stripes in the frequency domain. The FFM method has been implemented in the operational TROPOMI CO processor (V2.x.x). Additionally, to the uncorrected output, the user can now access the corrected TROPOMI CO columns and the destriping mask via the variable `carbonmonoxide_total_column_corrected` and `carbonmonoxide_total_column_stripe`. The FFD methods shows an even better destriping performance compared to the FFM method and is considered for future updates of the operational processing.

### 4.2 Solved Data Quality Issues

#### QA value (solved in version 01.02.02)

Sun glint is wrongly considered in the calculation of the `qa_value`. This is corrected since the activation of version 01.02.02 (December 2018, see Table 2).

#### Orbit numbering in NRTI and OFFL (solved in version 01.02.02)

Note that NRTI orbit numbers are set with respect to the downlink orbit while OFFL orbit numbers are set with respect to the equator crossing time. This creates an inconsistency between the NRTI and OFFL orbit numbers, which is removed with the activation of processor version 01.02.02 (December 2018, see Table 2).

#### Metadata/Attributes (solved in version 02.02.00)

The spatial resolution of the TROPOMI measurements is improved by bringing the along track ground pixel size from 7.0 to 5.5 Km starting on 6<sup>th</sup> August 2019. Note that, after this operations change, the metadata/Attributes fields related to the spatial resolution remained **unchanged** (hence not aligned to the improved resolution). These fields have been updated with the activation of Level 2 processors version 02.02.00.

#### Metadata values exchanged (solved)

The global attributes `geospatial_lon_min` and `geospatial_lon_max` values are exchanged; therefore, the user is advised to switch the values for these fields, making note that the `geospatial_lat_min` and `geospatial_lat_max` values are correct. This is an issue traceable to L1b data (version 01.00.00) and is corrected since the switch to version 02.00.00 of the Level 1B processor switched on July 2021.

#### Geolocation co-added when they should not be (solved in version 02.03.01)

In version 02.02.00, the geolocation of pixels near the pole show a shift of up to 300 meters due to a co-addition activity performed by mistake. This has been corrected in version 02.03.01.

### 4.3 Data Features

This section describes some characteristics of the data that might seem anomalous, however they are physically correct and not related to any problem.

### **Pixel geolocation around North Pole (feature)**

The solar irradiance is measured on a daily basis over the North Pole at a reference azimuth angle to remove seasonal effects on the measurements. To this end, a yaw manoeuvre is executed when the instrument is still in radiance mode, causing possible distortion on the scanlines observed during this manoeuvre (i.e. crossing scanlines, "bow-tie" ground pixel shape instead of rectangular). This occurs at most during the last 26 seconds of radiance measurements every 15<sup>th</sup> orbit (once every 25 hours). Though this may seem anomalous, it is physically correct, and not related to any problem on the data geolocation.

### **4.4 Mission Operations Changes**

A change in the Copernicus Sentinel 5P operations scenario increasing the spatial resolution from 7.0 km to 5.5 km along track for all measurements, became operational starting from 6 August 2019, orbit 9388.

## **5 Algorithm Change Record**

For a detailed description of the L2\_\_CO\_\_\_\_ algorithms, please refer to the ATBD [RD02].

## 6 Data Format

The product is stored as NetCDF4 file. The NetCDF4 file contains both the data and the metadata for the product.

For OFFL data the product is stored as a single file per satellite orbit, for NRTI data the product is stored as multiple files per orbit.

Please note that consecutive data granules of the NRTI product show an overlap of about 12 scan lines.

Details of the data format are provided in the Product User Manual (PUM) [RD03].

### 6.1 Data format changes

#### 6.1.1 Version 02.04.00

##### New fields added

/PRODUCT/SUPPORT\_DATA/INPUT\_DATA/carbonmonoxide\_profile\_apriori contains the TMS profile *a priori* used for the profile scaling retrieval.

/METADATA/QA\_STATISTICS/number\_of\_thermal\_instability\_warning\_occurrences

In variable:

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/processing\_quality\_flags

Added element to attribute 'flag\_meanings': [success, radiance\_missing, irradiance\_missing, input\_spectrum\_missing, ..., **thermal\_instability\_warning**]

Added element to attribute 'flag\_masks': [255, 255, 255, ..., **1073741824**]

Added element to attribute 'flag\_values': [0, 1, 2, 3, 4, ..., **1073741824**]

##### Unit change of a field

/PRODUCT/DETAILED\_RESULTS/column\_averaging\_kernel attribute unit changed from the unit (m) to its unit less representation (1).

#### 6.1.2 Version 02.03.01

There are no format changes with respect to the previous version.

#### 6.1.3 Version 02.02.00

##### New fields added

/METADATA/QA\_STATISTICS attribute number\_of\_missing\_scanlines

/METADATA/QA\_STATISTICS attribute number\_of\_max\_num\_outlier\_exceeded\_error\_occurrences

/METADATA/GRANULE\_DESCRIPTION attribute CollectionIdentifier

/PRODUCT/carbonmonoxide\_total\_column\_corrected: This variable contains the carbon monoxide total column with a destriping correction applied. The destriping algorithm requires a full orbit, and is therefore not possible in NRTI processing. In a NRTI granule this variable only contains fill values.

/PRODUCT/SUPPORT\_DATA/DETAILED\_RESULTS/carbonmonoxide\_total\_column\_stripe\_offset: This variable is the stripe correction (offset) that is calculated in OFFLINE processing.

##### Removed fields

/METADATA/ISO\_METADATA/gmd:identificationInfo/gmd:spatialResolution

##### Renamed fields

/PRODUCT/qa\_value attribute valid\_min\_

→ /PRODUCT/qa\_value **attribute** valid\_min

/PRODUCT/qa\_value **attribute** valid\_max\_

→ /PRODUCT/qa\_value **attribute** valid\_max

/METADATA/QA\_STATISTICS **attribute** number\_of\_aai\_warning\_occurrences

→ /METADATA/QA\_STATISTICS **attribute** number\_of\_AAI\_warning\_occurrences

#### **6.1.4 Version 01.04.00**

There are no format changes with respect to the previous version.

#### **6.1.5 Version 01.03.00**

##### **New fields added**

/PRODUCT/SUPPORT\_DATA/INPUT\_DATA/eastward\_wind

/PRODUCT/SUPPORT\_DATA/INPUT\_DATA/northward\_wind

## 7 Product Availability

All S5P/TROPOMI data are available on the Copernicus Open Data Hub <https://scihub.copernicus.eu>.

The list of major mission data gaps due to acquisition faults or satellite/instrument disruption is available at <https://sentinel.esa.int/web/sentinel/missions/sentinel-5p/mission-status>. For those periods the data are permanently lost.

Information on data handling tools is available from the web page <http://www.tropomi.eu/tools>.

For further questions regarding S5P/TROPOMI data products please contact [EOSupport@Copernicus.esa.int](mailto:EOSupport@Copernicus.esa.int).

The access and use of any Copernicus Sentinel data available through the Copernicus Sentinel Data Hub is governed by the Legal Notice on the use of Copernicus Sentinel Data and Service Information and is given here:

[https://sentinels.copernicus.eu/documents/247904/690755/Sentinel\\_Data\\_Legal\\_Notice](https://sentinels.copernicus.eu/documents/247904/690755/Sentinel_Data_Legal_Notice).

## 8 References

- [RD01] Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase  
**source:** ESA; **ref:** ESA-EOPG-CSCOP-PL-0073;  
**url:** <https://sentinels.copernicus.eu/documents/247904/2474724/Sentinel-5P-Calibration-and-Validation-Plan.pdf>
- [RD02] Algorithm Theoretical Baseline Document for Sentinel-5 Precursor: Carbon Monoxide Total Column Retrieval,  
**source:** SRON **ref:** SRON-S5P-LEV2-RP-002,  
**url:** <https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-Carbon-Monoxide-Total-Column-Retrieval>
- [RD03] Sentinel-5 precursor/TROPOMI Level 2 Product User Manual Carbon Monoxide  
**source:** KNMI; **ref:** SRON-S5P-LEV2-MA-002;  
**url:** <https://sentinels.copernicus.eu/documents/247904/2474726/Sentinel-5P-Level-2-Product-User-Manual-Carbon-Monoxide>
- [RD04] Borsdorff, T., aan de Brugh, J., Schneider, A., Lorente, A., Birk, M., Wagner, G., Kivi, R., Hase, F., Feist, D. G., Sussmann, R., Rettinger, M., Wunch, D., Warneke, T., and Landgraf, J.: Improving the TROPOMI CO data product: update of the spectroscopic database and destriping of single orbits, *Atmos. Meas. Tech.*, 12, 5443–5455, <https://doi.org/10.5194/amt-12-5443-2019>, 2019.
- [RD05] Borsdorff, T., Hasekamp, O. P., Wassmann, A., and Landgraf, J.: Insights into Tikhonov regularization: application to trace gas column retrieval and the efficient calculation of total column averaging kernels, *Atmos. Meas. Tech.*, 7, 523–535, <https://doi.org/10.5194/amt-7-523-2014>, 2014.
- [RD06] Algorithm theoretical basis document for the TROPOMI L01b data processor  
**source:** KNMI; **ref:** S5P-KNMI-L01B-0009-SD;  
**url:** <https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMI-Level-1B-ATBD>

More information on this data product is available from the Sentinel product webpage:

<https://sentinels.copernicus.eu/web/sentinel/technical-guides/sentinel-5p/products-algorithms>,

and from the corresponding TROPOMI product webpage <http://www.tropomi.eu/data-products>.

## Abbreviations and acronyms

ATBD	Algorithm Theoretical Basis Document
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
CAMS	Copernicus Atmosphere Monitoring Service
CO	Carbon Monoxide
DOI	Digital Object Identifier
ESA	European Space Agency
ESL	Expert Support Laboratory
ESRIN	European Space Research Institute
FFD	Fourier Filter Destriping
FFM	Fixed masked destriping Method
FTIR	Fourier Transform Infra-Red
IFS	ECMWF Integrated Forecasting System
KNMI	Royal Netherlands Meteorological Institute / Koninklijk Nederlands Meteorologisch Instituut
MOPITT	Measurements of Pollution in the Troposphere
MPC	Mission Performance Centre
NDACC	Network for the Detection of Atmospheric Composition Change
NRTI	Near Real Time
OFFL	Offline
PRF	Product Readme File
PUM	Product User Manual
ROCVR	Routine Operations Consolidated Validation Report
RPRO	Reprocessing
S5P	Sentinel-5 Precursor
S5PVT	Sentinel-5 Precursor Validation Team
SEOMS-IAS	Scientific Exploitation of Operational Missions – Improved Atmospheric Spectroscopy Databases
SZA	Solar Zenith Angle
TCCON	Total Carbon Column Observing Network
TROPOMI	Tropospheric Monitoring Instrument
VDAF	Validation Data Analysis Facility