COPS PDS L2-TO-L4 DATA PROCESS

Documentation

Abstract

This document contains the description of the software converting the COPS PDS CODMAC L2 to L4

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1. PURPOSE

The COmet Pressure Sensor (COPS) is calibrated relative to molecular nitrogen N_2. It is therefore necessary to correct the densities measured by COPS with the ratios of the molecules which are actually measured by COPS. These ratios are provided by the Double Focusing Mass Spectrometer (DFMS) instrument.

This document describes the conversion of the COPS PDS level 2 (L2) into PDS level 4 (L4), using the DFMS PDS level 3 (L3) data.

2. METHOD OVERVIEW

2.1. Method Description

For each COPS PDS level 2 data product, the closest non-GCU high resolution DFMS PDS level 3 spectra containing the major species (H_2O, CO, O_2, and CO_2) and some minor species (CH_4, NH_3, HCN, H_2CO, C_2H_6, CH_3OH, H_2S, C_2H_5OH, OCS, CS_2) detected by DFMS are found and integrated numerically. If one or more of these species cannot be found within a time span of 2 hours, the COPS PDS level 2 file is ignored. From the ratios of these species to H_2O, and knowing the sensitivities and fragmentation patterns for these molecules thanks to calibration campaigns on the ground with the laboratory replica of the two mass spectrometers, the total absolute local densities for each COPS PDS level 2 timestamps are computed using the corrected COPS Nude Gauge (NG) PDS level 2 pressure values.

The output consists of one .LBL file plus one .ASC file per molecule, for each MTP. A description of the .ASC and .LBL file formats is provided in the ".FMT" files corresponding to the COPS PDS level 4. The .ASC files include a time stamp, some information regarding the geometry of the Rosetta spacecraft, the total COPS density with its error, the COPS PDS level 2 filename, and the four DFMS PDS level 3 filenames used for the density values calculations.

COPS PDS level 4 are generated starting MTP6, as no or very few cometary data are available in the preceding data.

2.2. Method Process

The step-by-step overview of the conversion from one COPS PDS level 2 data file to its corresponding entry/line in the PDS level 4 output data files is described hereafter.

1. Read the relevant DFMS PDS level 3 data files: for each file, store the acquisition time and compute the amount of ions/s for the major and minor species (H_2O, CO, O_2, CO_2, CH_4, NH_3, HCN, H_2CO, C_2H_6, CH_3OH, H_2S, C_2H_5OH, OCS, and CS_2).

2. Read the COPS NG and BG PDS level 2 data files: for each file, store the acquisition time together with the pressure value.

3. Find the DFMS PDS level 3 data (for each species) closest in acquisition time to each COPS NG and BG PDS level 2 file and correct the COPS data with the DFMS ratios (see section 3.4).

4. Write the output to the PDS level 4 file.

Details on these steps are given in the Chapter 3 of this document. The tree architecture of the COPS PDS level 4 files is as follows:

```
[COPS L4 main folder]
    > MTP2
        > COPS
            … [COPS PDS level 4 data] …
    > MTP3
        > COPS
            … [COPS PDS level 4 data] …
    > MTP4
        …
```

3. DATA PROCESSING

3.1. COPS density values

The COPS pressure values needed for the computation of the corrected densities are extracted from the COPS NG and BG PDS level 2 files on line 117 ("ROSINA_COPS_PRESSURE_NG").

3.2. Numerical integration of the major and minor species

The species used for the scaling of COPS are H_2O, CO, O_2, CO_2, CH_4, NH_3, HCN, H_2CO, C_2H_6, CH_3OH, H_2S, C_2H_5OH, OCS, and CS_2. The species' ratios to H_2O are computed from the non-GCU high-resolution DFMS MCP PDS level 3 spectra.

The numerical integration of the major species in the DFMS spectra is done as follows:

1. The DFMS PDS level 3 data products are read until a spectrum corresponding to H_2O, CO, O_2, CO_2, CH_4, NH_3, HCN, H_2CO, C_2H_6, CH_3OH, H_2S, C_2H_5OH, OCS, or CS_2 is found.

2. The peak corresponding to the ongoing molecule is found while searching for the highest point near the theoretical mass of the said molecule. The possible values for the theoretical masses are summarized in the table below. These theoretical masses are calculated using the Commission on Isotopic Abundances and Atomic Weights (CIAAW) database; the mass of an electron has been subtracted.

H_2O^+	18.0100161	H_2CO^+	30.0100161
CO^+	27.9943660	$C_2H_6^+$	30.0464016
O_2^+	31.9892807	CH_3OH^+	32.0256662
CO_2^+	43.9892807	H_2S^+	33.9871727
CH_4^+	16.0307516	$C_2H_5OH^+$	46.0413162
NH_3^+	17.0260005	OCS^+	59.9664372
HCN^+	27.0103505	CS_2^+	75.9435938

3. The points are summed up on the left side of the peak centre, and then on the right side, each time until the next value becomes negative (end of the peak), or until the next value becomes higher than the previous ones (possible start of neighbouring peak).

If the four major species (at least) are not found within a time span of 2 hours, the COPS PDS level 4 data point is discarded.

3.3. COPS and DFMS acquisition times

The acquisition time for a COPS PDS level 2 file is defined as being the STOP_TIME value minus 5 seconds. The STOP_TIME is available in the header of each COPS PDS level 2 file (line 33).

The acquisition time for a DFMS PDS level 3 file is defined as the mean value between the START_TIME and the STOP_TIME. The START_TIME and STOP_TIME are available in the header of the DFMS PDS level 3 file (lines 42 and 43 respectively).

3.4. Scaling the ion counts/s with COPS

The calculations hereafter are based on the fact that the density measured by COPS is calibrated relative to molecular nitrogen N_2. Assuming that the coma is dominated by the major and minor species defined above, the COPS density is equal to the following sum:

$$n_{\mathrm{COPS}} = \frac{n_{\mathrm{H_2O}}}{\beta_{\mathrm{H_2O}}} + \frac{n_{\mathrm{CO}}}{\beta_{\mathrm{CO}}} + \frac{n_{\mathrm{O_2}}}{\beta_{\mathrm{O_2}}} + \frac{n_{\mathrm{CO_2}}}{\beta_{\mathrm{CO_2}}} + \frac{n_{\mathrm{CH_4}}}{\beta_{\mathrm{CH_4}}} + \frac{n_{\mathrm{NH_3}}}{\beta_{\mathrm{NH_3}}} + \frac{n_{\mathrm{HCN}}}{\beta_{\mathrm{HCN}}} + \frac{n_{\mathrm{H_2CO}}}{\beta_{\mathrm{H_2CO}}} + \frac{n_{\mathrm{C_2H_6}}}{\beta_{\mathrm{C_2H_6}}} + \frac{n_{\mathrm{CH_3OH}}}{\beta_{\mathrm{CH_3OH}}} + \frac{n_{\mathrm{H_2S}}}{\beta_{\mathrm{H_2S}}} + \frac{n_{\mathrm{C_2H_5OH}}}{\beta_{\mathrm{C_2H_5OH}}} + \frac{n_{\mathrm{OCS}}}{\beta_{\mathrm{OCS}}} + \frac{n_{\mathrm{CS_2}}}{\beta_{\mathrm{CS_2}}}$$

where β is a scale factor relative to N_2, reflecting the different ionization probabilities. Values below are from the Granville-Phillips User Manual (2007) for the major species (H_2O, CO, O_2, and CO_2) and calculated based on the ionization cross sections at 150 eV for the other species:

$\beta_{\mathrm{H_2O}}$	$= 0.893$	$\beta_{\mathrm{CH_4}}$	$= 0.654$	$\beta_{\mathrm{C_2H_6}}$	$= 0.380$	β_{OCS}	$= 0.532$
β_{CO}	$= 0.952$	$\beta_{\mathrm{NH_3}}$	$= 0.787$	$\beta_{\mathrm{CH_3OH}}$	$= 0.541$	$\beta_{\mathrm{CS_2}}$	$= 0.207$
$\beta_{\mathrm{O_2}}$	$= 0.990$	β_{HCN}	$= 0.645$	$\beta_{\mathrm{H_2S}}$	$= 0.455$		
$\beta_{\mathrm{CO_2}}$	$= 0.704$	$\beta_{\mathrm{H_2CO}}$	$= 0.631$	$\beta_{\mathrm{C_2H_5OH}}$	$= 0.335$		

Total uncorrected COPS density is defined as:

$$n_{\mathrm{COPS}} = 2.45 \cdot 10^{22} \cdot p_{\mathrm{COPS}}$$

with n_{COPS} the COPS NG total density in m^{-3} (not species corrected), and p_{COPS} the COPS NG pressure in mbar. After switch-on, COPS densities are higher due to filament outgassing. Normally, it is best to ignore data taken within half an hour from switch-on and also ignore data during slews >5° or somewhat larger later in the mission at close distances. In addition, COPS was not always switched-off during WOL's, especially later in the mission it was operated. This can

very well be seen, as COPS then reacts to the WOL with a sharp peak. COPS also reacts to dust impact, seen by fast (a few minutes) peaks. In addition, during enhanced solar activity, COPS can react to energetic ions, leading to "noise" on the measured density.

Individual densities for the mass spectrometer DFMS are defined as:

$$n_i = \frac{a \frac{c_i}{Y_i}}{S_i f_{i \to j}}$$

with
i: index representing one of the species
a: constant including all parameters that are sensor dependent but independent of the species
c_i: number of ions/sec (yield corrected) on detector for species i
Y_i: species and sensor dependent yield for species i
S_i: species, sensor, and emission dependent sensitivity
$f_{i \to j}$: species and sensor dependent fragmentation ratio

We now define the ratios of the densities relative to H_2O, which are independent of any degradation of the sensors (a vanishes):

$$r_{O_2} = \frac{n_{O_2}}{n_{H_2O}} = \frac{\frac{c_{O_2}}{Y_{O_2}} S_{H_2O} f_{H_2O \to H_2O^+}}{\frac{c_{H_2O}}{Y_{H_2O}} S_{O_2} f_{O_2 \to O_2^+}}$$

$$r_{CO_2} = \frac{n_{CO_2}}{n_{H_2O}} = \frac{\frac{c_{CO_2}}{Y_{CO_2}} S_{H_2O} f_{H_2O \to H_2O^+}}{\frac{c_{H_2O}}{Y_{H_2O}} S_{CO_2} f_{CO_2 \to CO_2^+}}$$

… and so on for the other species, except for CO and H_2CO. The contribution from CO_2 to the CO signal needs to be subtracted as follows (the same applies for the contribution of CH_3OH to H_2CO):

$$r_{CO} = \frac{n_{CO}}{n_{H_2O}} = \frac{\left(\frac{c_{CO}}{Y_{CO}} - \frac{c_{CO_2}}{Y_{CO_2}} \frac{f_{CO_2 \to CO^+}}{f_{CO_2 \to CO_2^+}}\right) S_{H_2O} f_{H_2O \to H_2O^+}}{\frac{c_{H_2O}}{Y_{H_2O}} S_{CO} f_{CO \to CO^+}}$$

Table 1 summarizes the numerical values used for S_i, f_i, and Y_i.

Table 1: summary of the sensitivity (S), fragmentation (f_1 & f_2), and yield (Y) values, for DFMS (MC).

Species	*S [cm³]*	f_1		f_2		*Y*
H_2O	$2.302 \cdot 10^{-19}$	H_2O^+	0.7919			0.885
CO	$2.028 \cdot 10^{-19}$	CO^+	0.9638			1.420
O_2	$1.583 \cdot 10^{-19}$	O_2^+	0.8210			1.623
CO_2	$1.537 \cdot 10^{-19}$	CO_2^+	0.7791	CO^+	0.0991	2.141
CH_4	$8.671 \cdot 10^{-19}$	CH_4^+	0.5220			0.790
NH_3	$4.576 \cdot 10^{-19}$	NH_3^+	0.4750			0.837
HCN	$3.124 \cdot 10^{-19}$	HCN^+	0.7920			1.367
H_2CO	$3.187 \cdot 10^{-19}$	H_2CO^+	0.3090			1.525
C_2H_6	$2.294 \cdot 10^{-19}$	$C_2H_6^+$	0.1060			1.526
CH_3OH	$6.897 \cdot 10^{-19}$	CH_3OH^+	0.1300	H_2CO^+	0.0300	1.624
H_2S	$0.705 \cdot 10^{-19}$	H_2S^+	0.5740			1.717
C_2H_5OH	$3.132 \cdot 10^{-19}$	$C_2H_5OH^+$	0.0300			2.232
OCS	$1.294 \cdot 10^{-19}$	OCS^+	0.5280			3.044
CS_2	$10.35 \cdot 10^{-19}$	CS_2^+	0.6640			2.590

With the ratios defined above, one can finally derive the species' densities:

$$n_{\mathrm{H_2O}} = \frac{n_{\mathrm{COPS}}}{\frac{1}{\beta_{\mathrm{H_2O}}} + \frac{r_{\mathrm{CO}}}{\beta_{\mathrm{CO}}} + \frac{r_{\mathrm{O_2}}}{\beta_{\mathrm{O_2}}} + \frac{r_{\mathrm{CO_2}}}{\beta_{\mathrm{CO_2}}} + \frac{r_{\mathrm{CH_4}}}{\beta_{\mathrm{CH_4}}} + \frac{r_{\mathrm{NH_3}}}{\beta_{\mathrm{NH_3}}} + \frac{r_{\mathrm{HCN}}}{\beta_{\mathrm{HCN}}} + \frac{r_{\mathrm{H_2CO}}}{\beta_{\mathrm{H_2CO}}} + \frac{r_{\mathrm{C_2H_6}}}{\beta_{\mathrm{C_2H_6}}} + \frac{r_{\mathrm{CH_3OH}}}{\beta_{\mathrm{CH_3OH}}} + \cdots}$$

$$n_{\mathrm{CO}} = r_{\mathrm{CO}}\, n_{\mathrm{H_2O}}$$

$$n_{\mathrm{O_2}} = r_{\mathrm{O_2}}\, n_{\mathrm{H_2O}}$$

$$n_{\mathrm{CO_2}} = r_{\mathrm{CO_2}}\, n_{\mathrm{H_2O}}$$

… and so on for the minor species, again in densities of m^{-3}. After switch-on, COPS densities used in the normalization process are higher due to filament outgassing. Normally, it is best to ignore data taken within half an hour from switch-on and also ignore data during slews >5° or somewhat larger later in the mission at close distances. In addition, COPS was not always switched-off during WOL's, especially later in the mission it was operated. This can very well be seen, as COPS then reacts to the WOL with a sharp peak. COPS also reacts to dust impact, seen by fast (a few minutes) peaks. In addition, during enhanced solar activity, COPS can react to energetic ions, leading to "noise" on the measured density.

3.5. Error on the densities

Due to the errors on the COPS density (ca. 7%), on the DFMS sensitivity factors (ca. 16%), and on the DFMS fragmentation factors (ca. 10%), the total estimated error for the total COPS density numbers is set to 20%.

3.6. LBL files

In addition to the .ASC files (i.e. the PDS level 4 containing the time series of the COPS density values), a .LBL file is available for each MTP. These .LBL files contain information about the corresponding .ASC file such as the product ID, the data set ID, the size… An example is given on the next page, copied from the COPS PDS level 4 from MTP33.

Example: **COPS_L4_MTP33.LBL**

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PDS_VERSION_ID·····================·····PDS3·····¶
LABEL_REVISION_NOTE·····==========·····"2018-01-24,Thierry·Semon(UoB)"·····¶
RECORD_TYPE·····==================·····FIXED_LENGTH·····¶
RECORD_BYTES·····=================·····626·····¶
FILE_RECORDS·····=================·····26350·····¶
^COPS_TS_TABLE·····===============·····"COPS_L4_MTP33.ASC"·····¶
PRODUCT_ID·····===================·····COPS_L4_MTP33·····¶
PRODUCT_CREATION_TIME·····========·····2019-04-11T12:21:03·····¶
PROCESSING_LEVEL_ID·····==========·····"4"·····¶
DATA_SET_ID·····==================·····"RO-C-ROSINA-4-EXT3-V1.0"·····¶
DATA_SET_NAME·····================·····"ROSETTA-ORBITER·67P·ROSINA·4·····¶
·····EXT3·V1.0"·····¶
TARGET_NAME·····==================·····"67P/CHURYUMOV-GERASIMENKO·1·(1969·R1)"¶
TARGET_TYPE·····==================·····"COMET"·····¶
MISSION_NAME·····=================·····"INTERNATIONAL·ROSETTA·MISSION"·····¶
MISSION_PHASE_NAME·····===========·····"ROSETTA·EXTENSION·3"·····¶
INSTRUMENT_HOST_NAME·····=========·····"ROSETTA-ORBITER"·····¶
INSTRUMENT_HOST_ID·····===========·····RO·····¶
INSTRUMENT_NAME·····==============·····"ROSETTA·ORBITER·SPECTROMETER·FOR·····¶
·····ION·AND·NEUTRAL·ANALYSIS"·····¶
INSTRUMENT_ID·····================·····ROSINA·····¶
INSTRUMENT_MODE_ID·····===========·····"N/A"·····¶
^INSTRUMENT_MODE_DESC·····========·····"COPS_MODE_DESC.ASC"·····¶
DETECTOR_ID·····==================·····COPS·····¶
CHANNEL_ID·····===================·····"N/A"·····¶
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STOP_TIME·····====================·····2016-09-02T06:36:44·····¶
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SPACECRAFT_CLOCK_STOP_COUNT·····=·····"1/431418916.05330"·····¶
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SC_TARGET_POSITION_VECTOR·····===·····"N/A"·····¶
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SUB_SPACECRAFT_LONGITUDE·····=====·····"N/A"·····¶
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·····"DE405.BSP",·····¶
·····"ROS_V32.TF",·····¶
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                                    "ROS_160929_STEP.TSC",
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                                    "CORB_DV_257_03___T19_00345.BSP",
                                    "RORB_DV_257_03___T19_00345.BSP",
                                    "RATT_DV_257_02_01_T6_00344.BC"}
OBJECT                          =   COPS_TS_TABLE
   NAME                         =   COPS_TS_TABLE
   INTERCHANGE_FORMAT           =   ASCII
   ROWS                         =   26350
   COLUMNS                      =   25
   ROW_BYTES                    =   626
   ^STRUCTURE                   =   "COPS_TS_TABLE.FMT"
END_OBJECT                      =   COPS_TS_TABLE
END
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