ROSINA PDS L3-TO-L5 DATA PROCESS
Documentation

Abstract
This document contains the description of the software converting the DFMS and RTOF PDS CODMAC L3 to L5

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1

Contents

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1. PURPOSE

This document describes the process required to convert the Double Focusing Mass Spectrometer (DFMS) and the Reflectron-type Time-Of-Flight (RTOF) PDS level 3 (L3) into PDS level 5 (L5), using the COmet Pressure Sensor (COPS) PDS level 2 data for normalization.

2. METHOD OVERVIEW

2.1. Method Description

For each mass spectrometer's non-GCU level 3 data product, the ion count of the major species are integrated. These species consist of H_2O, and CO_2 for RTOF, and of 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 for DFMS. From the ratios of each 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 absolute local densities are computed using the corrected COPS Nude Gauge (NG) density as absolute reference.

The output consists of one .LBL file plus one .ASC file per molecule, for each MTP, and for each instrument. A description of the .ASC and .LBL file formats is provided in the ".FMT" files corresponding to the DFMS & RTOF PDS level 5. The .ASC files include a time stamp, some information regarding the geometry of the Rosetta spacecraft, the local density of each molecule with its error, the PDS level 3 filenames used for the density values calculations (1 for RTOF, 14 for DFMS), the total COPS density, and the filename of the COPS PDS level 2 file used for the absolute scaling with COPS.

PDS level 5 are generated starting MTP6, as no or very few cometary data are available in the preceding data. The DFMS PDS level 5 data after 2016-09-05 18:00 (mid-MTP 34 & MTP 35) are not provided neither due to a dust event that occurred at that time and that considerably lowered the sensitivity of the instrument, making the interpretation of the data more complex. Finally, no RTOF PDS level 5 data are available in the MTP 21 and 35, due to the absence of RTOF PDS level 3 data for these time periods.

2.2. Method Process

The step-by-step overview of the conversion from one PDS level 3 data file to its corresponding entry/line in the PDS level 5 output data files is given below. In the following, "MS" refers either to RTOF or to DFMS.

1. Read the relevant MS PDS level 3 data files: for each file, store the acquisition time and compute the amount of ions/s for the all the species.

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

3. For each RTOF PDS level 3 file: find the COPS PDS level 2 file closest in acquisition time to the RTOF PDS level 3 file.
   For each DFMS PDS level 3 containing one of the species: find the COPS PDS level 2 file closest in acquisition time to the DFMS level 3 file, and find the 13 other DFMS PDS level 3 files containing the other species.

4. Normalize the MS data to COPS (see section 3.4).

Details on these steps are given in the Chapter 3 of this document. The tree architecture of the PDS level 5 files is as follows:

```
[L5 main folder]
    > MTP2
        > DFMS
            … [DFMS PDS level 5 data] …
        > RTOF
            … [RTOF PDS level 5 data] …
    > MTP3
        > DFMS
            … [DFMS PDS level 5 data] …
        > RTOF
            … [RTOF PDS level 5 data] …
    > MTP4
        …
```

3. DATA PROCESSING

3.1. Numerical integration of the species

3.1.1. DFMS

The species processed in the DFMS PDS level 5 products are separated into the major species (H_2O, CO, O_2, and CO_2) and the minor species (CH_4, NH_3, HCN, H_2CO, C_2H_6, CH_3OH, H_2S, C_2H_5OH, OCS, and CS_2).For the numerical integration, only the non-GCU high-resolution DFMS MCP spectra are used.

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

1. The DFMS PDS level 3 data products are read until a spectrum corresponding to a major or to a minor species 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).

3.1.2. RTOF

For RTOF, the processed species are H_2O and CO_2. Unlike DFMS, CO and O_2 are excluded due to the more complex interpretation of the signal on masses 28 and 32 respectively, where other species could contribute to the intensity of the peak. The minor species are not extracted neither from the RTOF data due to lower sensitivity of RTOF to these less abundant minor species. The RTOF PDS Level 3 GCU spectra are ignored in the calculation of the PDS level 5 data.

The peak shape of a molecule in a time-of-flight mass spectrum can be approximated in a first approach to a Gaussian, $A\,e^{\left(-(x-x_0)^2\middle/2\sigma^2\right)}$, with σ increasing with the mass following a linear function. In the specific case of RTOF aboard Rosetta, we have:

$$\sigma = 0.003635 \cdot mass$$

Additionally, a baseline between the peaks exists due to several instrumental effects (such as electronic noise). The intensity of this baseline may vary from one spectrum to another, and is calculated by summing all the points between bin number 6500 and bin number 8000; this number is then divided by 1500, thus giving a background value per bin.

The integration consists in summing all the points between (*mass* - 2σ) and (*mass* + 2σ), where the background value described above is subtracted for each bin. The possible values for *mass* are 18.0100 (H_2O) and 43.9893 (CO_2). These theoretical masses are calculated using the Commission on Isotopic Abundances and Atomic Weights (CIAAW) database; the mass of an electron has been subtracted.

In case a data point in the RTOF PDS level 3 file would have a negative value before the background subtraction (e.g. value "-1" due to the *electronic noise correction* from the PDS level 2 to level 3 conversion), the point is discarded.

3.2. COPS, DFMS, and RTOF 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 or RTOF 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 each MS PDS level 3 file.

3.3. Finding the closest COPS value

Due to the fact that some COPS NG values were set to 0 (especially during the PRELANDING phase) because of wrong / missing offset measurements, an iterative process is followed to determine the most suitable COPS value to assign to a MS data point.

While processing one MS PDS level 3 spectrum, the COPS NG pressure value that has the closest acquisition time must be found.
- If this pressure value is not 0, then it is associated to the MS value.
- Otherwise, the second closest COPS NG pressure value is found.
    - o If this pressure value is not 0, then it is associated to the MS value.
    - o Otherwise, the MS PDS level 3 is discarded, and no entry for this file will be written in the PDS level 5 product.

If one or more of the four species cannot be found in a time range of +/- 2h, the COPS PDS level 2 file is ignored and no corresponding PDS level 5 data entry is created for this time period.

3.4. Finding the closest DFMS values

For DFMS, unlike RTOF where all the species are visible in each single spectrum, at least the four closest H_2O, CO, O_2, and CO_2 PDS level 3 spectra are necessary. If one or more of the four species is not found within a time span of 2 hours, the data point is discarded.

3.5. 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 (values in brackets are valid only for the DFMS process):

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

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:

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

Total uncorrected COPS density is defined as:

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

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 spectrometers DFMS & RTOF 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 H₂O, 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 H₂CO. The contribution from CO₂ to the CO signal needs to be subtracted as follows (the same applies for the contribution of CH₃OH to H₂CO):

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

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

Table 1: summary of the sensitivity (S), fragmentation (f₁ & f₂), and yield (Y) values, for DFMS (MC).

Species	S [cm³]	f₁		f₂		Y
H₂O	2.302 · 10⁻¹⁹	H₂O⁺	0.7919			0.885
CO	2.028 · 10⁻¹⁹	CO⁺	0.9638			1.420
O₂	1.583 · 10⁻¹⁹	O₂⁺	0.8210			1.623
CO₂	1.537 · 10⁻¹⁹	CO₂⁺	0.7791	CO⁺	0.0991	2.141
CH₄	8.671 · 10⁻¹⁹	CH₄⁺	0.5220			0.790
NH₃	4.576 · 10⁻¹⁹	NH₃⁺	0.4750			0.837
HCN	3.124 · 10⁻¹⁹	HCN⁺	0.7920			1.367
H₂CO	3.187 · 10⁻¹⁹	H₂CO⁺	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:

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

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

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

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

… 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.

3.6. Error on the densities

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

3.7. LBL files

In addition to the .ASC files (i.e. the PDS level 5 containing the time series of the DFMS & RTOF density values), a .LBL file is available for each MTP and for each molecule. 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 RTOF PDS level 5 for H_2O (MTP34).

Example: `RTOF_L5_MTP34_H2O.LBL`

```
PDS_VERSION_ID                  =    PDS3
LABEL_REVISION_NOTE             =    "2018-01-24,Thierry Semon(UoB)"
RECORD_TYPE                     =    FIXED_LENGTH
RECORD_BYTES                    =    194
FILE_RECORDS                    =    2302
^RTOF_TS_TABLE                  =    "RTOF_L5_MTP34_H2O.ASC"
PRODUCT_ID                      =    RTOF_L5_MTP34_H2O
PRODUCT_CREATION_TIME           =    2019-03-31T19:26:59
PROCESSING_LEVEL_ID             =    "5"
DATA_SET_ID                     =    "RO-C-ROSINA-5-EXT3-V2.0"
DATA_SET_NAME                   =    "ROSETTA-ORBITER 67P ROSINA 5
                                     EXT3 V2.0"
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           =    "RTOF_MODE_DESC.ASC"
DETECTOR_ID                     =    RTOF
CHANNEL_ID                      =    "N/A"
START_TIME                      =    2016-09-02T11:17:14
STOP_TIME                       =    2016-09-25T16:26:45
SPACECRAFT_CLOCK_START_COUNT    =    "1/431435745.28015"
SPACECRAFT_CLOCK_STOP_COUNT     =    "1/433441516.35685"
SC_SUN_POSITION_VECTOR          =    "N/A"
SC_TARGET_POSITION_VECTOR       =    "N/A"
SC_TARGET_VELOCITY_VECTOR       =    "N/A"
SPACECRAFT_ALTITUDE             =    "N/A"
SUB_SPACECRAFT_LATITUDE         =    "N/A"
SUB_SPACECRAFT_LONGITUDE        =    "N/A"
SPICE_FILE_NAME                 =    {"NAIF0011.TLS",
                                     "DE405.BSP",
                                     "ROS_V32.TF",
                                     "ROS_CHURYUMOV_V01.TF",
                                     "ROS_160929_STEP.TSC",
                                     "CATT_DV_257_03_____00344.BC",
                                     "CORB_DV_257_03___T19_00345.BSP",
                                     "RORB_DV_257_03___T19_00345.BSP",
                                     "RATT_DV_257_02_01_T6_00344.BC"}
OBJECT                          =    RTOF_TS_TABLE
   NAME                         =    RTOF_TS_TABLE
   INTERCHANGE_FORMAT           =    ASCII
   ROWS                         =    2302
   COLUMNS                      =    13
   ROW_BYTES                    =    194
   ^STRUCTURE                   =    "RTOF_TS_TABLE.FMT"
END_OBJECT                      =    RTOF_TS_TABLE
END
```