ROSETTA ROSINA

ROSINA

User's Guide

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1.0	12.06.2019	All	First Issue
1.1	19.08.2019	All	Add Acronyms paragraph, add text to chapter 3.10

Acronyms

DFMS   Double Focussing Mass Spectrometer

DPU   Digital Processing Unit

GCU   Gas Calibration Unit

ID   Identification

HV   High Voltage

MCP   Multichannel plate

MS   Mass Spectrometer

MTP   Medium Term Planning

PA   Post Acceleration

PPM   Pulse Position Modulation

RTOF   Reflection-type Time-Of-Flight Mass Spectrometer

S/C   Spacecraft

SW   Software

UoB   University of Bern

WOL   Wheel Offloading

ROSINA User's Guide

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1. Purpose and a word of caution

The purpose of this document is a short description on how to use the publicly available ROSINA data in the PSA and PDS archives. It is intended to make the users of these data aware of the content of the archive, of the degree of data reduction for the different levels and of how these data can be used and how they should not be used.

A mass spectrometer is a complex instrument which involves quite a lot of physics and chemistry. ROSINA level 2 and 3 data, which are raw data and data with physical units, should therefore only be used by people familiar with mass spectrometry. Level 4 (COPS density data) and level 5 (density of specific parent molecules as a function of time) can in principle be used by "everybody" familiar with the Rosetta mission / its trajectory as long as some caution is applied because S/C motion (see below).

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2. The art of mass spectrometry

There are different approaches to how species can be identified, be it in solid or in gaseous form. Looking directly at the mass/charge ratio of a species is called mass spectrometry. In order to do this, one has to separate species with different masses/charge ratios. The ROSINA instrument suite uses two different principles. The classical approach is by ionising the species, accelerating them and then applying electrical and magnetic fields for spatial separation according to their mass. The precision of this approach depends on the mechanical precision of the ion optical elements. This technique is used in DFMS. A more novel approach is to accelerate ionised species to a fixed energy and then measure the time of flight between the ion source and the detector as this is then mass dependent. The mass resolution here is given by the time resolution of the detector electronics as well as the time focusing properties of the ion optics. This approach is used in RTOF.

In both cases the first step is always ionisation of neutral species. This is done with electron impact ionisation, whereby the electrons are generated by a hot Tungsten-Rhenium filament. This process ionises species, but at the same time also fragments molecules. The ionization cross section is specific for each molecule / atom and depends on the energy of the impacting electrons. The so called fragmentation pattern depends on the electron energy as well, but in addition to that also on the mass dependent analyser section of the instrument and on the specifics of the detector yield. A typical fragmentation pattern is given in fig. 1 for propane. In principle, fragmentation patterns for all species have to be calibrated beforehand with the instrument. This was impossible for ROSINA, as most species were unknown before launch. The ROSINA team is calibrating as many species as possible even now with the flight-like models in the lab and the fragmentation patterns can be found in the archive. However, there are species which are either too poisonous or too corrosive to be handled safely. For these species an alternate approach is to use fragmentation patterns found in literature, while being aware that they might easily differ by a factor 2 or more from the specific ROSINA sensor.

Fig. 1: fragmentation pattern for propane (C_3H_8) in DFMS

When identifying species it is mandatory to check fragmentation. If a fragment is missing in the spectrum, then your identification is wrong (false positive detection)!

3. DFMS

3.1. Applicable documents

Details on the ROSINA-DFMS sensor can be found in:

a. Balsiger, H., Altwegg, K., Bochsler, P., Eberhardt, P., Fischer, J., Graf, S., ... & Müller, J. (2007). Rosina–Rosetta orbiter spectrometer for ion and neutral analysis. *Space Science Reviews*, *128*(1-4), 745-801.

b. ROSINA User Manual including appendix D1-DFMS instrument modes (part of the archive)

Details on the data analysis and uncertainty considerations can be found in:

a. Le Roy, L., Altwegg, K., Balsiger, H., Berthelier, J. J., Bieler, A., Briois, C., ... & Fiethe, B. (2015). Inventory of the volatiles on comet 67P/Churyumov-Gerasimenko from Rosetta/ROSINA. Astronomy & Astrophysics, 583, A1.

b. Calmonte, U., Altwegg, K., Balsiger, H., Berthelier, J. J., Bieler, A., Cessateur, G., ... & Gasc, S. (2016). Sulphur-bearing species in the coma of comet 67P/Churyumov–Gerasimenko. *Monthly Notices of the Royal Astronomical Society*, *462*(Suppl_1), S253-S273.

3.2. Short instrument description

DFMS is a classical magnetic mass spectrometer in the Nier-Johnson configuration with a variable electrostatic field and a permanent magnet. The main elements are: the ion source, the electrostatic analyser, the magnet, the zoom optics and the detectors. In neutral mode, the ion source is biased vs. S/C ground to 200V in order to repel positive ions. Negative ions get too much energy to pass the analyser. In ion mode, the ion source is on S/C ground or slightly negative to attract positive ions.

Ionisation is done with electron impact, electrons having 45 eV. The normal mode in space has an electron current of 200 μA. Ionised species are accelerated towards the electrostatic analyser. In order to pass either the high resolution slit (14μm) or the low resolution slit (200 μm) they are deflected by at least 7°. This prevents dust from settling on the slit. The ion source is an open source. Non-ionized species just pass through in order not to have chemistry in the ion source. The hot filament is hidden from the ionisation box for the same reason. Temperature in the ionisation box is monitored and is ~ few °C normally. In order to pass the electrostatic analyser, the energy has to be within 1% of the nominal energy for which the ESA is set up, as given by the acceleration voltage, which depends on the mass to be measured. The acceleration voltage has a 1/sqrt(m) dependence, that means it's ~-4760V for mass 13 and -617 V for mass 100. Low energy ions are more scattered in the sensor which leads to a mass-dependent sensitivity. Ions with the correct momentum pass the magnet. In high resolution, the zoom optics enlarges the image of the entrance slit by a factor of 6.4 for masses between 18 Da and 69 Da, somewhat less below 18 Da and above 70 Da (see below). After the zoom optics, ions hit the MCP-LEDA detector, consisting of a multi-channel plate and a

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linear detector array. The MCP is operated in an analogue mode where the gain (the voltage across the detector) is adjusted according to the signal strength. This allows for a high dynamic range of 10^{10}, but has the disadvantage that different masses are measured at different gain steps. Because masses above 69 Da have low energies where the MCP is no longer very sensitive, they are accelerated by an additional acceleration voltage PA of 1000 V just before the detector. This leads to a jump in all of the parameters (mass scale, dispersion, sensitivity) between mass 69 and 70 Da. Between masses 13 and 69, the sensitivity follows a $1/m^{0.8}$ law. The linear detector array behind the MCP collects the electrons with 2 rows of 512 pixels, each pixel being ~25 μm. DFMS normally measures in high resolution mode, one integer mass at the time, where the sensor is tuned to put this mass near the middle of the detector. To get a mass spectrum, the sensor has to be stepped through the mass range required. Integration time per mass is 20s, the overhead (switching of voltages, adjustment of the gain) needs about 10s.

3.3. The main operation modes

All operation modes for DFMS can be found in the ROSINA User Manual (appendix D1-DFMS instrument modes (part of the archive)).

DFMS could be operated in ion mode, where the filament was switched off and the ion source box was at S/C potential, or in neutral mode with the filament mostly on 200 μA electron emission and the ion source box at +200V. Within these two main types of modes, there are modes for high resolution (narrow entrance slit) and low resolution (broad entrance slit). Modes consisted then of measuring a certain mass range or mass selection by commanding a mode number. Mode numbers ending with 0 are low resolution modes, while those ending with 2 are high resolution modes. The most used mode was m222, which covers the mass range from m/z 13 to m/z 100 in high resolution. For each mode, m/z 18 was measured at the beginning and end of the mode, M222 therefore produced 90 mass spectra, each with the integer center mass near the middle of the detector. This means that a mode m222 lasts ~45 min. For ions, the most used mode was m320, a low resolution mode covering the mass range from 13 to 50.

3.4. L2, L3 and L5 data set description

L2 data is the raw data as received from the instrument. They contain some housekeeping and "science housekeeping" information followed by three rows giving the pixel number and ADC counts of row A and row B. The difference between housekeeping and "science housekeeping" is the timing. Science housekeeping are read out at the end of the spectrum. They therefore reflect the status at the stop time, but are only a selection and often consist only of flags ok/nok. Housekeeping data are read out regularly every minute. The closest housekeeping in time are added to the spectrum. As a spectrum takes only 30 s, housekeeping may therefore represent the status of the last spectrum or the next spectrum. All information necessary to determine mass scale and intensity are given in the science housekeeping. But it needs some experience to go from raw data to data with

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physical units. L2 spectra can contain irregularities. The most common is a byte shift which can be seen mostly in a jump of the offset values. In rare cases they may also contain a wrong mode number. DFMS produced about 2 million spectra over the mission which makes it impossible to check them by hand.

L3 data contain the same spectra as L2, but they have physical units whereby pixels are replace by m/z, and ADC counts by ions/s. Irregularities have been corrected where possible or the spectra deleted from L3 if correction was not possible. In the first version, the mass scale only contains 2 digits, e.g. mm.xx (18.01). The resolution of DFMS in high resolution mode is clearly better. This means there will be several pixels all containing the same m/z. This is done because the automatic analysis of data often has an uncertainty of ~0.01 Da. This is due to thermal effects of the instrument, especially of the magnet. In order to get a better mass scale we refer the reader to the next section. An improved version of L3 will contain 4 digits, but this takes time as much of the data has to be checked manually.

L5 data finally contain density data for as many species as possible for the whole mission as a function of time. For these data, mass peaks have been integrated, sensitivity and ionization cross section have been taken into account and the data have been cross-calibrated to COPS data. COPS is a very simple instrument with no ageing in sensitivity. The COPS data can therefore be used for an absolute calibration of the mass spectrometer data (see 5.7). L5 data can be used directly, plotted, integrated, etc. Normally, it is best to ignore data taken within half an hour after switching DFMS on and also any taken during slews >5°. However, these are local densities in the vicinity of the S/C and not production rates. Due to the special shape of 67P and the orbit of the S/C around the comet, a coma model has to be used to get production rates. Several models have been developed for 67P and can be found in literature. In addition, L5 data have to be taken with care around the switch-on time of the instrument or during slews as they may contain contaminants from the filament outgassing when switched on or from the S/C during slews.

3.5. How to establish a mass scale

3.5.1. Pixel0, dispersion, zoom

The mass scale can be calculated according to this formula:

$$m = m_0 \cdot \exp\left(\frac{(x - x_0) \cdot 25}{D \cdot z}\right)$$

eq. 1

With

- m   : mass
- m_0 : commanded mass
- x   : pixel on LEDA
- x_0 : pixel related to m_0
- z   : zoom factor (LR z = 1; HR z = 6.4)
- D   : dispersion constant (D=125'000 µm)
- 25 µm/px : conversion factor pixel to µm

X0 is called pixel0 and is the pixel where the theoretical mass m0 would have its centre. E.g. you command m/z=28.000. There is no molecule which actually has this exact mass, but if there were, it would centred on pixel0. z is the zoom factor which is 1 for low resolution mode and theoretically 6.4 for high resolution for masses between 18 and 69. The dispersion is constant.

However:

- This is only true for masses near the centre of the detector (pixel 256)
- x_0 is not a constant value (depends on T_{magnet} and m_0)
- z   may change slightly for HR
    - m13-m20: z ∈ [5.4;6.6]
    - m > m20: z~ 6.4 ± 0.4
    - influence of the post-acceleration (PA = -50V (LR und HR, m<70)
              PA = -1000V (HR, m>69))

In order to get x0 and possibly z you have to look at a peak where you know what it is (exact mass, at least 4 digits). According to eq. 1, you then calculate x0. X0 does not normally change more than 1 pixel between subsequent spectra except between mass 69 and 70, where you get a jump in pixel0 and in z due to the post-acceleration. You always have to make sure, that all assigned peak masses correspond to a real existing species fragment. There are no "fake" peaks. Especially for masses >69, where post-acceleration sets in, you need to know more than one peak mass per spectrum, as you also have to fit the zoom. An example is given below.
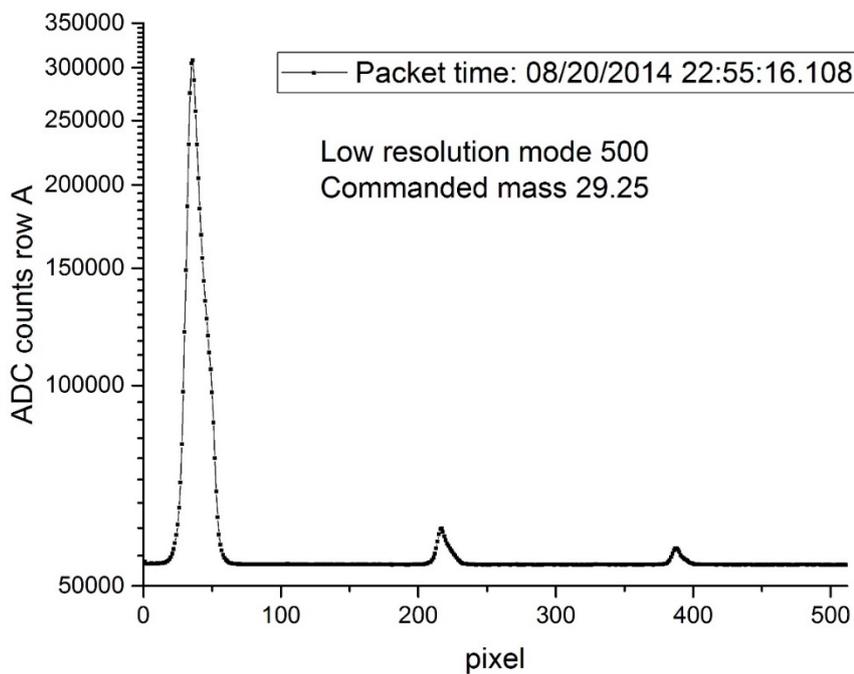
Fig. 2 : DFMS MCP Low resolution spectrum, raw data
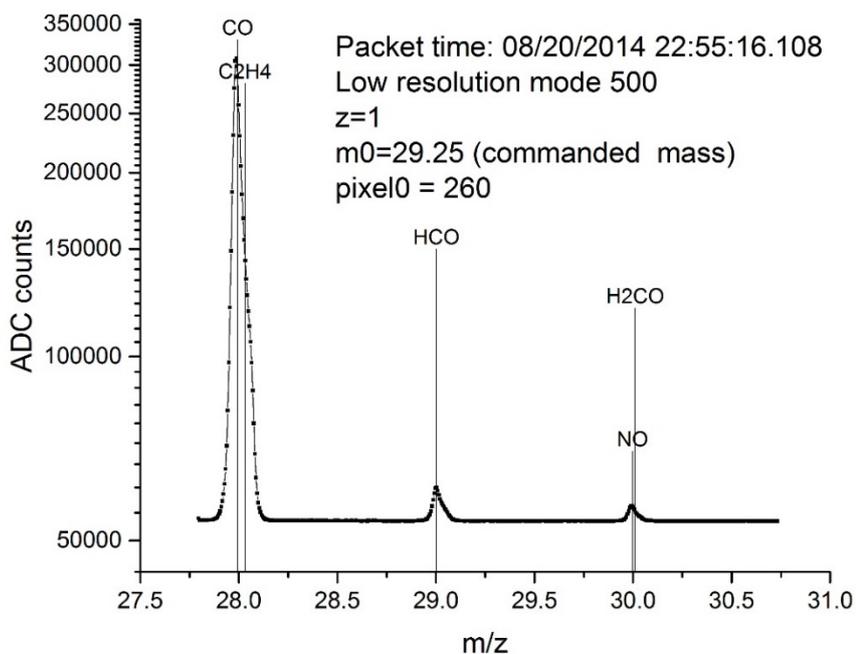
Fig 3 : DFMS MCP Low resolution spectrum with mass scale: m=29.250 * exp ((pixel-260)*25/125000×1)
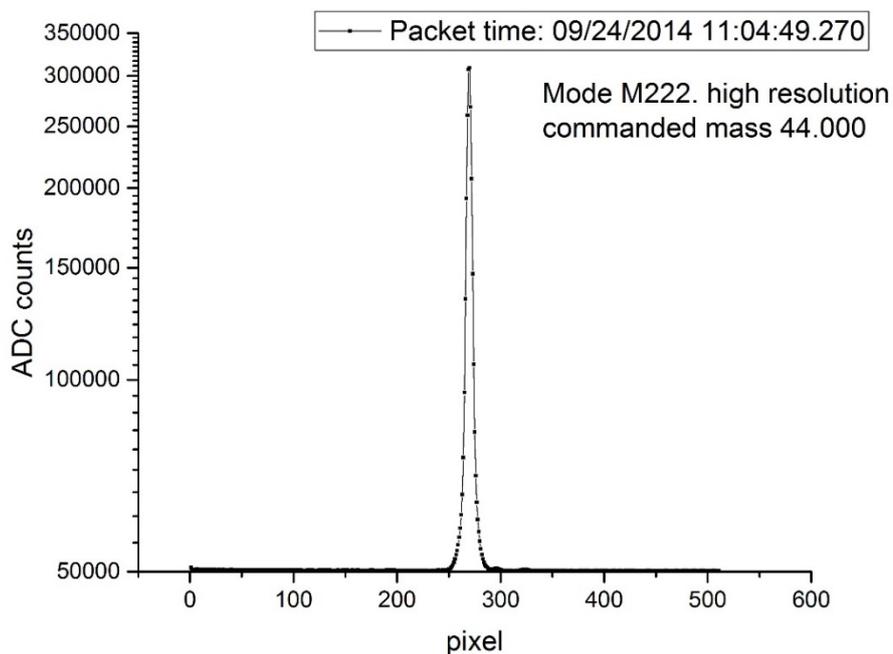
Fig. 4 DFMS MCP High resolution spectrum, commanded mass 44.000
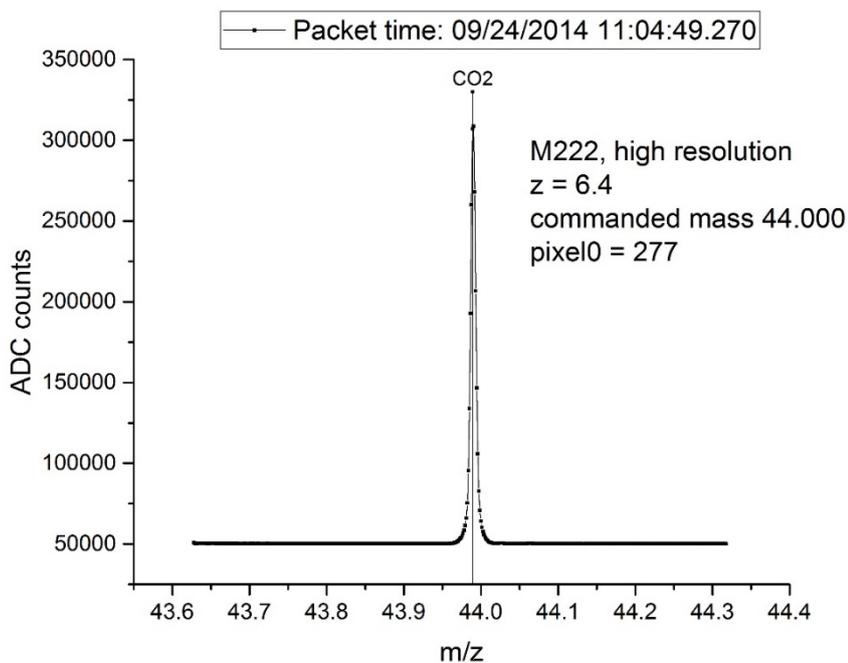
Fig.5: DFMS MCP High resolution spectrum with mass scale: $m = 44.000 * \exp((pixel-277)*25/125000 \times 6.4)$
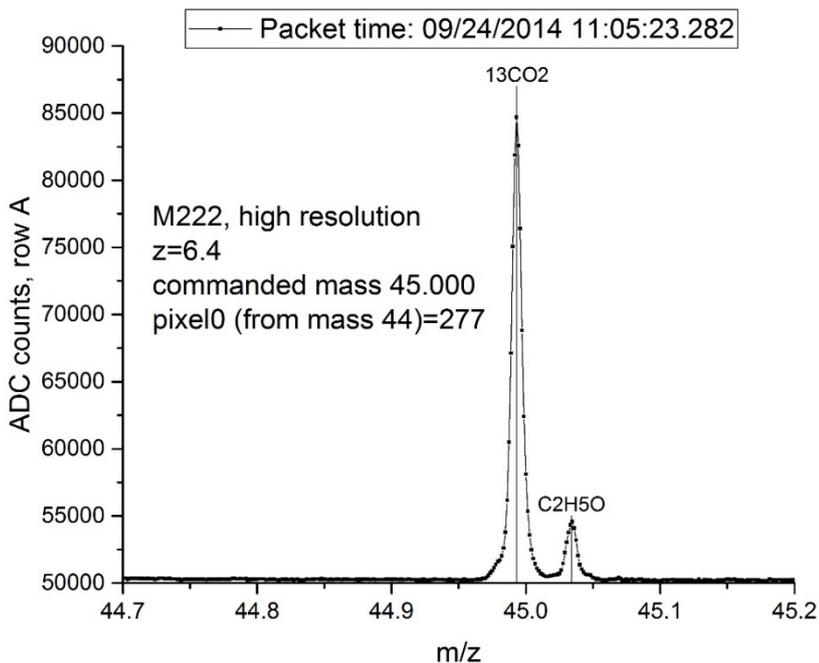
Fig.6 : DFMS MCP High resolution spectrum with mass scale: m=45.000 * exp ((pixel-277)*25/125000×6.4). Pixel0 was evaluated for mass 44.
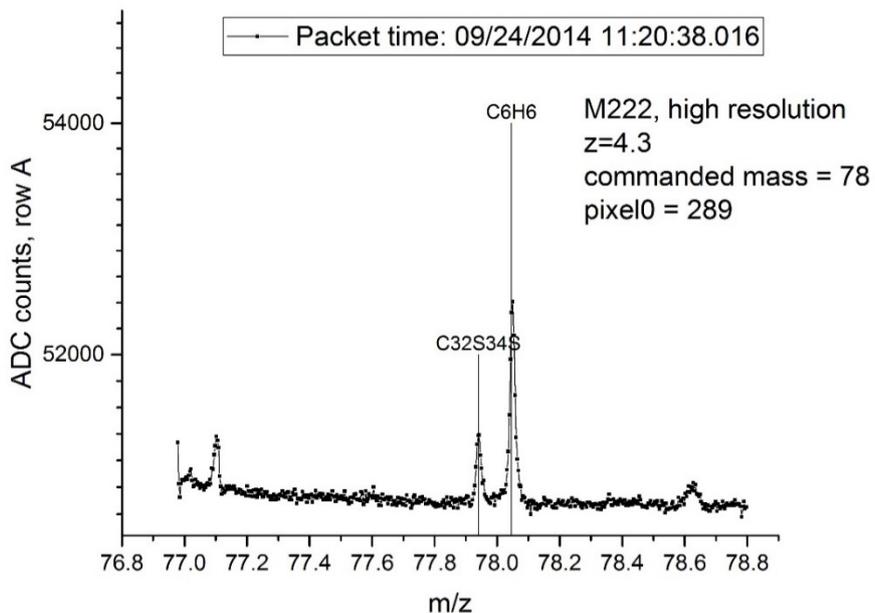
Fig.7: DFMS MCP High resolution spectrum with mass scale: m=78.000 * exp ((pixel-289)*25/125000×4.3). Zoom factor is now only 4.3 and the pixel0 has shifted due to the postacceleration.

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3.6. Row A and row B

The DFMS detector has two rows of 512 pixels each for redundancy reasons. They can be co-added to enhance the signal, or they can be used separately. Depending on the mission phase, row A or row B is normally more sensitive due to the electric field distribution in the ion source (contaminants). As the absolute density has to be scaled to COPS, this has no consequences. The mass peaks on the two rows can be shifted by up to three pixels. When co-adding, this has to be taken into account in the case where mass resolution is very important.

3.7. Mass dependent sensitivity and ionisation cross section

Because all ions need the same momentum to pass the permanent magnet, their energy is lower for higher masses. This leads to mass discrimination in the analyser section (lower energy means more scattering) and in the detector yield (lower ion energies produce less electrons in an MCP).. For masses < 70 Da the mass dependence of the sensitivity is $\sim 1/m^{0.8}$. In addition there is a dependence of the detector yield on the kind of species (atomic ions vs. large molecular ions). This has to be calibrated. The ionisation cross section of species is dependent on the electron energy.

If available, sensitivity and fragmentation data should be taken from the ROSINA archive. If not available, then a literature search for ionisation cross sections at 45 eV has to be done and the mass dependent sensitivity of the detector has to be taken into account.

In order to get physical units for the y-axis the following steps also have to be taken:

3.7.1. Offset subtraction

In order to operate the LEDA, it first has to be charged with a small charge which is then seen as the offset value. This offset is not constant over the detector and not the same for both rows. Normally the offset is fitted outside of the peak area with a polynomial (see fig. a-d below).
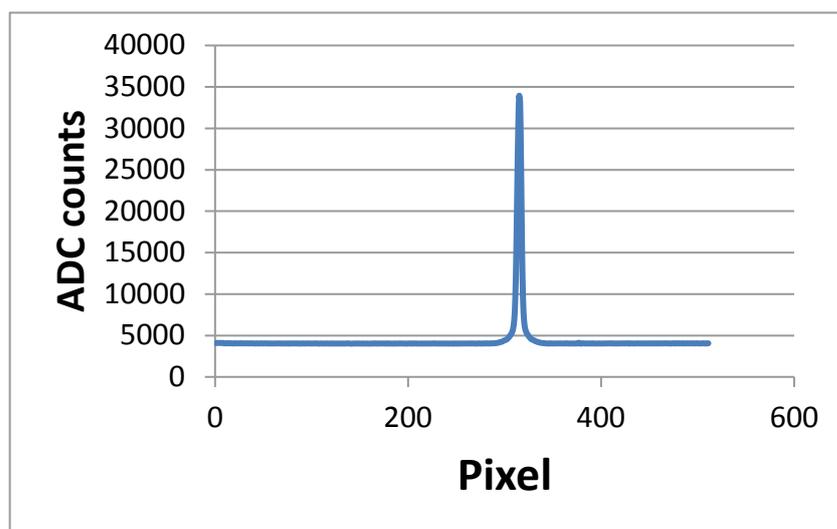
Fig. a: raw data
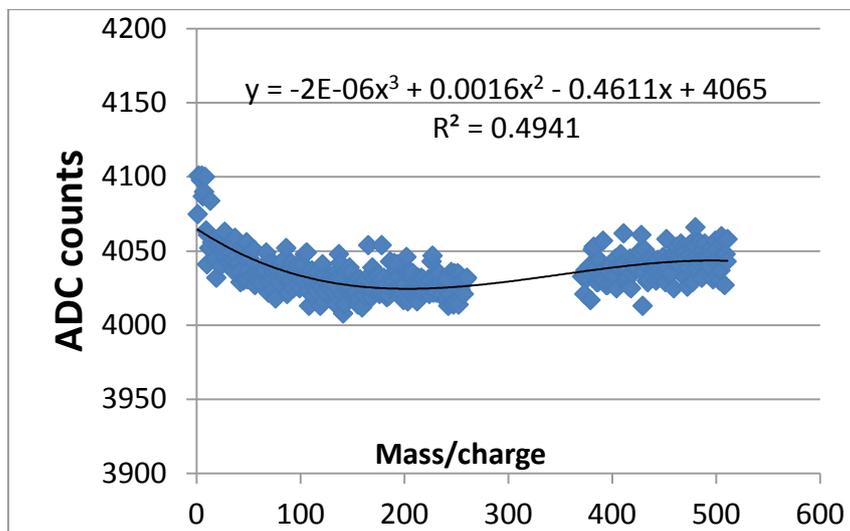
Fig. b: offset fitting outside of the peak area
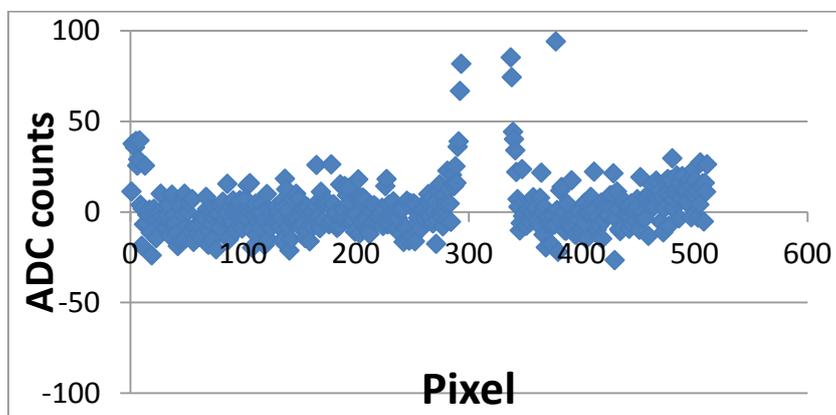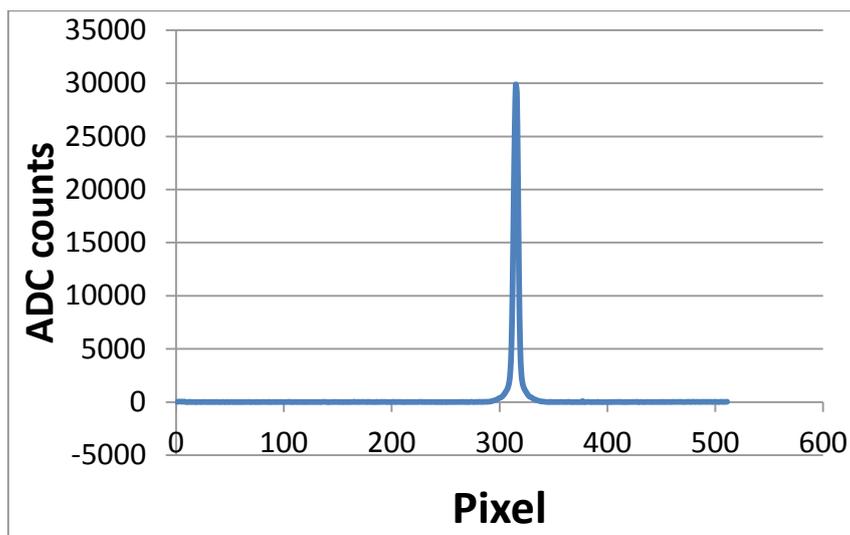
Fig. c+d: data after offset subtraction

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3.7.2. Calculation of ions/s

$$I_i(px) = \frac{ADCcounts(px)}{og * ig(px)} \frac{1}{y_s} \frac{conv_{ADC} c_{leda}}{t_{tot}} \quad [A]$$

eq. 2

With   ADCcounts(px):   # of counts on Pixel px

og: overall gain, in 16 steps, gain step given in the science housekeeping

ig(px):   individual pixel gain

y_s: detector yield for species s

$conv_{ADC}$:   conversion factor $= \frac{1}{2^{12}-1} \cdot 2.5V = 6.105e-4 \quad V$

c_{LEDA}:   4.22 pF

and I_i normalised to detector yield =1   (corresponds to N_2, 3000V)

#ions/s = I_i(px)/1.602e-19   eq. 3

The overall gain og (gain for each gain step) is given in the archive data and depends on the date because of detector ageing. An example is given below (before arrival at the comet):

Gain step	Gain
1	1.41E-01
2	3.88E-01
3	1.01E+00
4	2.79E+00
5	7.63E+00
6	2.20E+01
7	6.48E+01
8	1.94E+02
9	5.97E+02
10	1.90E+03
11	6.41E+03
12	2.25E+04
13	7.84E+04
14	2.89E+05
15	1.02E+06
16	2.78E+06

The individual pixel gain depends also on the date and on the pixel number. The individual pixel gain curves are given in the archive. For dates in between measured pixel gains, it is suggested to interpolate.
For an example see fig. e below:

79	....
80	0.729607
81	0.757114
82	0.779278
83	0.777076
84	0.755651
85	0.729921
86	0.708454
87	0.694484
88	0.676432
89	0.662922
90	0.660682
91	0.660673
92	0.667662
93	0.678242
94	0.699162
95	0.724082
96	0.738891
97	0.74975
98	0.76545
99	0.774541
100	0.775832
101	....
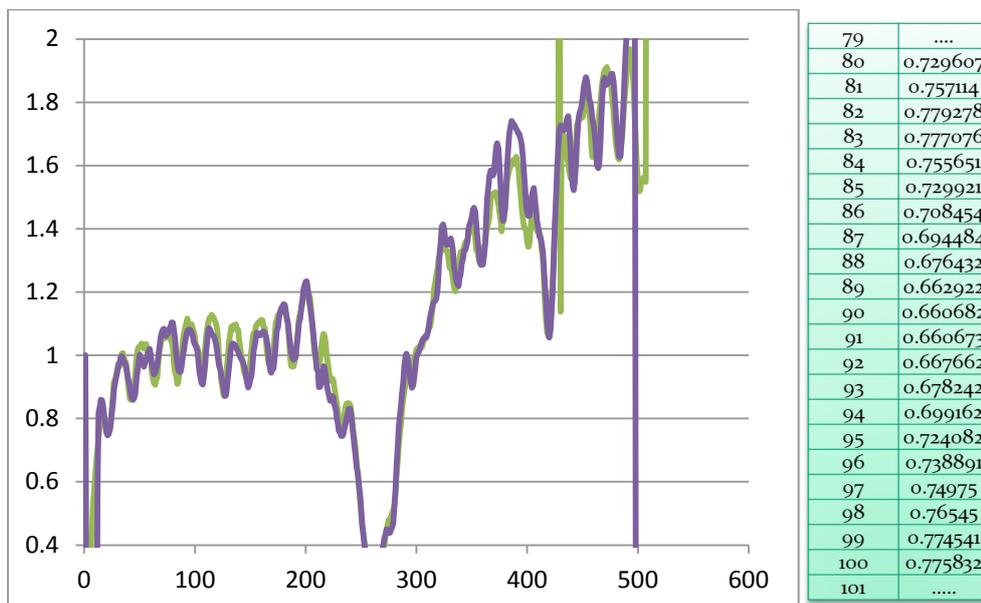
Fig. e: individual pixel gain (date: 2010)

Using the overall gain and the pixel gain, the integration time of 20s and the ADC counts per pixel, the spectrum shown above can then be transformed with eq. 2 and eq. 3 into the following spectrum with the y-axis in ions/s:
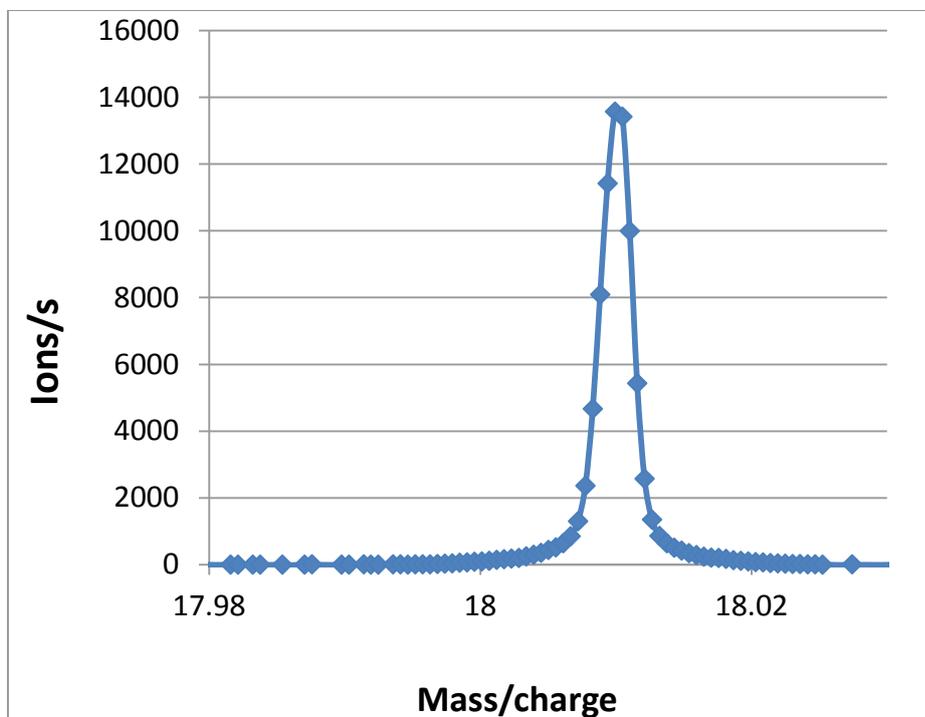
A short formula to get ions/s taking into account the energy dependent yield, but not the species dependent one is for masses <70:

#ions/s = $1/(0.00000044892*m^4 - 8.8158e{-5}*m^3 + 0.0064995*m^2 - 0.2223*m + 3.4922)/20*(ADC\_counts-OFFSET)*og(gain\ step)*ig(pixel,\ gain\ step)$

And for masses >69

#ions/s = 1/(0.5684-0.0024*m)*0.58e-2/20*(ADC_counts-OFFSET)*og(gain step)*ig(pixel, gain step)

3.7.3. Total number of ions

In order to get the area under peak, ions can be summed up in the case of a single peak, or a fitting function can be used. The best result is given by a pseudo Voigt (fig. f, example below) or by two Gaussian with the same centre, but different width. The two Gaussian approach is only necessary for low signals below 10% of the main peak as the height of the second Gauss is <10% of the first. If two peaks have a similar height, then 1 Gaussian curve for each of them is normally sufficient (fig. g). The peak width over the MCP does not change and has therefore to be fixed to one value applicable to all species present.

Modell	PsdVoigt2		
Gleichung	y = y0 + A * (mu * (2/PI) * (wL / (4*(x-xc)^2 + wL^2)) + (1 - mu) * (sqrt(4*ln(2)) / (sqrt(PI) * wG)) * exp(-(4*ln(2)/wG^2)*(x-xc)^2))		
Chi-Quadr Red uziert	2162.0236		
Kor. R-Quadrat	0.99846		
		Wert	Standardfehler
B	y0	-7.66994	2.2982
B	xc	18.01005	1.57044E-4
B	A	47.52384	0.29749
B	wG	0.00252	1.63396E-5
B	wL	0.00523	5.95373E-4
B	mu	0.31227	0.01802

Fig.f: Pseudo Voigt

Fitparameters:
$H^{18}O$: 19.007 fixed
$H_2^{17}O$: 19.01478 fixed
HDO: 19.01684 fixed
Y0: 1150
FWHM: 0.00362 fixed
Areas:
$H^{18}O$: 12.3
$H_2^{17}O$: 14.1
HDO: 11.61

-> D / ^{17}O = 0.41
Literature SMOW: 0.4099

Fig. g: Several species on m/z = 19. The width for the Gaussian curve can be deduced from the left peak (^{18}OH) and then applied to the two species hidden behind the right peak ($H_2^{17}O$ and HDO). With the known masses for these two species, the only fit parameters remaining are the heights.

3.7.4. Density of species j

Fragmentation

- Molecules are dissociated/ionised by electron impact.
- Fragmentation pattern depends on electron energy.
- Fragmentation patterns are instrument dependent. It is not correct to take patterns for example from the NIST without being aware of the uncertainties attached to this!
- For DFMS the nominal electron energy is 45eV.
- The fragmentation tables in the archive contain the parent and all non-zero daughters.
- The numbers are normalised to the highest peak (100%) which is not necessarily the parent (analog to the NIST tables).

Ionisation cross sections for different species can be found in literature, but be aware of the uncertainties!

Literature on ionisation cross section shows large variability in the results, e.g.
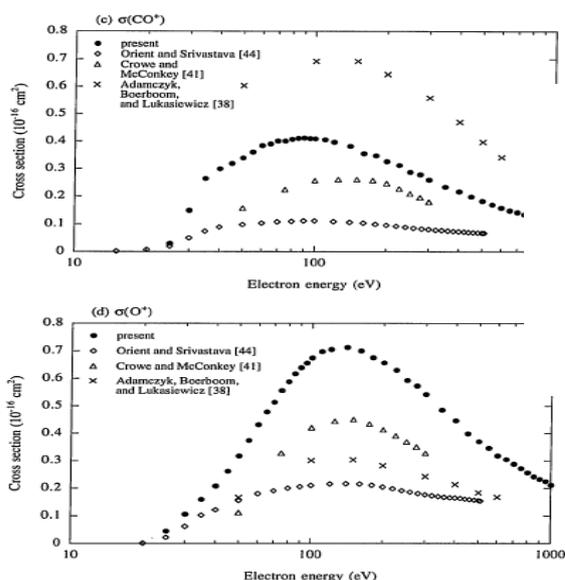
Fig. h: Different Ionization cross sections for CO2 into CO$^+$ and O$^+$ from the PhD thesis of HC Straub.

Sensitivity:

$$S = Cs\,(I_e)*tau*yield$$

With

Cs(I_e): cross section (function of electron current, electron energy and species)
tau: transfer function (function of energy and resolution)
yield: detector yield relative to N2, 3000V (function of energy and species)

Sensitivities for calibrated compounds can be found in the archive.

3.7.5. Calculating densities

a)   From fragments

$$I_i\,(\mu A) = I_e\,(\mu A)\,S_j\,(cm^3)\,Q_{ij}\,n_j\,(cm^{-3})$$

Ie: electron current
Sj: Sensitivity for gas j
Qij :   Fragmentation pattern for ion species i of gas j e.g. O$^+$ from CO^2
n$_j$:   density in cm^{-3} for species j

b)   From the parent species

$$I_{main}\,(\mu A) = I_e(\mu A)\,S_{parent}\,(cm^3)\,n(cm^{-3})$$

S_{parent} Sensitivity for parent species (can be found in the archive or approximated from literature and the energy dependence of the instrument's mass-dependent sensitivity (see above)). A good description on how to get approximations from literature for unmeasured sensitivities can be found in *Le Roy, L., Altwegg, K., Balsiger, H., Berthelier, J. J., Bieler, A., Briois, C., ... & Fiethe, B. (2015). Inventory of the volatiles on comet 67P/Churyumov-Gerasimenko from Rosetta/ROSINA. Astronomy & Astrophysics, 583, A1.*

3.8. Ion modes, energy dependence

For ions, ionisation cross sections do not come into play as these are primary ions from the coma being measured. However, DFMS was built to measure thermal ions inside of the ionosphere of the comet. As the spacecraft was never really inside this ionosphere, ions have non-thermal energies. The sensitivity of DFMS however is strongly dependent on the energy. The acceptable range of the electrostatic analyser is +/- 1% of the nominal energy. Because heavier masses must have lower nominal energies in order to pass the permanent magnet, their energy windows are smaller than for lighter ions: e.g. the energy window for water ions is ~34 eV, whereas for CO_2 it is only 14 eV. If the S/C is negatively charged, ions will have energies in this range, even if they are thermal ions. It is therefore almost impossible to calculate real ion densities.

3.9. Using COPS data for the absolute calibration

As described above, detector ageing of the MCP plays a major role. While the relative gain between pixels was measured regularly throughout the mission (pixel gain files in the archive) and the relative overall gain between gain steps could be assessed after the mission by looking at the fragmentation pattern of water, which is supposed to stay constant, the absolute overall gain cannot be measured in flight. However, this can be overcome by using COPS data for calibration, as it measures absolute densities. For a description on how to calibrate DFMS data with COPS see chapter 5.7.

3.10.   Pitfalls, irregularities

High resolution mass spectrometry is an "art" and DFMS was a very complex instrument. There are many pitfalls, some of which are mentioned below:
- A small offset in the pixel0 can lead to a totally "different" comet, especially for higher masses. There are many species which have very similar m/z, differing by less than 0.001 Da. Using the wrong species can distort the whole deduced composition of the comet.

- A check which should always be done is the H_n check. Species which contain several hydrogen atoms usually produce fragments with H_n, H_{n+1}, H_{n+2}.... These are shifted relative to their integer masses by 0.008 Da. This pattern can be easily recognised.

- Species which don't contain hydrogen are always less than (on the left side of) the integer mass, e.g. CO_2 at m/z=43.997.

- Look for isotopologues. If you detect something with ^{35}Cl, you should always also see its isotopologue at ^{37}Cl.

- In January 2016, the nominal pixel0 was shifted by 50 pixels towards lower values because of detector ageing. Preceding this permanent shift, the change of the pixel0 was experimented with for short periods. This leads to jumps in pixel0.

- DFMS has a redundant filament. This was tested in spring 2016 so as to be prepared for a fast switch should filament 1 fail. It was never used, but in the data there are files with filament 2 used related to this test.

- Due to the many slews of the S/C, DFMS spectra are affected by contamination from sublimating gas from the S/C. Sudden jumps in intensity can therefore be the outcome of a slew.

- After being switched on, the instrument always needs some time to outgas the filament and to get into thermal equilibrium. Therefore always look at the data in context, not at single spectra.

- Dust impacts affect mass spectra in DFMS as well as COPS intensities. They can be recognised by sudden increases in the COPS density followed by a slower decrease.

- Because DFMS is a very complex instrument, there were sometimes errors in the housekeeping data. In some cases this led to an immediate switch-off of the sensor, as the SW first had to decide if it was a transmission error or an actual hardware failure. There was never a real hardware failure, but such events are seen in the data as modes which were halted in the middle of execution. The instrument would then wait for the next command to resume operation. There are thus unexpected data gaps.

- Some transmission errors, known as byte-shifts, also occur in the science data and are seen as sudden jumps in the offset. In L3 data these errors have been corrected wherever possible or the files have been removed.

- Row B has a regular pattern in its offset which can be corrected for by using the formula ADC_counts = ADC_counts +(-1^{pixel_nr}*45), which adds / subtracts 45 from alternate pixels.

The ROSINA archiving team spent a lot of effort to detect and correct wrongly labeled data files. The most frequent error were wrong mode numbers in the label. This is due to a glitch in the DPU which changed sometimes the mode number to the next mode, although the current mode was not yet finished. The reason was a limited stack. Because DFMS has taken more than $2 \cdot 10^6$ individual spectra, it was impossible to check all spectra manually. We know that a few spectra may have slipped the

thorough automatic check done on the L2 and L3 data. We therefore recommend that in case you encounter some weird spectra, which do not fit the mode number (low resolution instead of high, ion mode instead of neutral mode, etc.) you look at the corresponding L2 spectrum and check some housekeeping, which will tell you immediately if there is a mismatch between mode number and real mode:

"ROSINA_DFMS_FIL_EMISSION   ","200uA","

neutral mode (filament emitting),

"ROSINA_DFMS_FIL_EMISSION   "," "0uA"

ion mode (no electrons emitted)

"ROSINA_DFMS_ZOOM_QUAD1   ","   ","191.2471 ","V"

high resolution (zoom on)

"ROSINA_DFMS_ZOOM_QUAD1   ","   ","xxx.xxxx ","V"   xxx<100

low resolution (zoom off)

4. RTOF

4.1. Applicable documents

Details on the ROSINA-RTOF sensor can be found in:

c. Balsiger, H., Altwegg, K., Bochsler, P., Eberhardt, P., Fischer, J., Graf, S., ... & Müller, J. (2007). Rosina–Rosetta orbiter spectrometer for ion and neutral analysis. *Space Science Reviews*, *128*(1-4), 745-801.

d. ROSINA User Manual including appendix D2-RTOF instrument modes (part of the archive)

Details on the data analysis and uncertainty considerations can be found in:

c. Gasc, S., Altwegg, K., Fiethe, B., Jäckel, A., Korth, A., Le Roy, L., ... & Wurz, P. (2017). Sensitivity and fragmentation calibration of the time-of-flight mass spectrometer RTOF on board ESA's Rosetta mission. *Planetary and space science*, *135*, 64-73.

4.2. Short instrument description

RTOF is a time of flight mass spectrometer. It contains two instruments in one, sharing some ion optical elements. Neutrals entering the sensor are ionised in a storage source where ions are stored for a short time. They are then extracted with a fast HV pulse and accelerated to a nominal energy of 1000 eV. After ~1m of flight time they are slowed down and reflected by a reflectron and then accelerated again to an energy of 1000 eV. Close to where they started, they hit the detector, where their time of arrival is registered. This part is called the SS (storage source). Species entering the orthogonal ion source (OS) are ionised and then immediately extracted orthogonally to their incoming velocity. They are accelerated and reflected as in the SS and hit the OS detector, where again their time of arrival is registered. The OS part is less sensitive as ions are only extracted if they happen to be at the right position at the time of the extraction pulse.

4.3. The main operation modes

i. OS
ii. SS

4.4. L2, L3 and L5 data set description

L2 data are raw data as received from the instrument. They contain some housekeeping and three rows with bin number, events and ADC counts. Housekeeping data are read out regularly every minute, which is compatible with the integration time of RTOF (200s). The closest housekeeping in time are added to the spectrum. All information necessary to determine mass scale and intensity are given in the housekeeping. But it needs some experience to go from raw data to data with physical units. L2 spectra can contain irregularities.

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L3 data contain the same spectra as L2, but they have physical units whereby pixels are replace by m/z, and ADC counts by ions/s. Irregularities have been corrected where possible or the spectra have been deleted from L3 if correction was not possible. In the first version, the mass scale only contains 2 digits, e.g. mm.xx (18.01). This corresponds to the resolution of RTOF. An improved version of L3 will contain 4 digits, but this takes time as much of the data has to be checked manually.

2. L5 data contain density data for as many species as possible for the whole mission as a function of time. For these data, mass peaks have been integrated, sensitivity and ionisation cross section have been taken into account and the data have been calibrated to COPS data. COPS is a very simple instrument with no ageing in sensitivity. The COPS data can therefore be used for an absolute calibration of the mass spectrometer data (see 5.7). L5 data can be used directly, plotted, integrated, etc.. Normally, it is best to ignore data taken within half an hour from switch-on and also ignore data during slews >5°. However, these are local densities in the vicinity of the S/C and not production rates. To get production rates a coma model has to be used, due to the special shape of 67P and due to the orbit of the S/C around the comet. Several models have been developed for 67P and can be found in literature.

4.5. CORRECTING THE "RAW" INPUT L2 DATA SIGNAL

Electronic noise

A pattern due to electronic noise is visible in many spectra and is corrected by setting all the points around specific bin values to a negative intensity (i.e. a central bin + the previous 48 bins + the following 48 bins are set to -1). This electronic pattern may be seen in the figure at the end of section 4.2. Several configurations exist, depending on the time period to be converted. The lists of the central bins are given below:

10kHz spectra – configuration 1 (MTP2 & MTP4):

3865, 4310, 4986, 5428, 10455, 12248, 13366, 14491, 15208, 21758, 22877, 24717, 25840, 26511, 27639, 34232

10kHz spectra – configuration 2 (MTP3 & MTP5):

3262, 3892, 4409, 5052, 5565, 6206, 6725, 7365, 7882, 8525, 9055, 9685, 10235, 10455, 10992, 11621, 12248, 12767, 13404, 13930, 14565, 15208, 15720, 16358, 16868, 17513, 18024, 18663, 19184, 19822, 20342, 20930, 21758, 22140, 22640, 22925, 24060, 24717, 25210, 25888, 26511, 27021, 27677, 28168, 28829, 29329, 29971, 30484, 31126, 31643, 32277, 32789, 33440, 33960, 34232, 34600

10kHz spectra – configuration 3 (MTP19 to MTP24):

3310, 3923, 4484, 5107, 5650, 6266, 6805, 7434, 7972, 8603, 9136, 9773, 10308, 10455, 11017, 11621, 12248, 12812, 13414, 13980, 14606, 15208, 15772, 16398, 16948, 17568, 18109, 18733, 19289, 19905, 20467, 21075, 21758, 22235, 22785, 22925, 24115, 24717, 25285, 25888, 26511, 27076, 27677, 28243, 28874, 29414, 30046, 30584, 31211, 31748, 32377, 32914, 33545, 34095, 34232, 34725

10kHz spectra – configuration 4 (all other MTPs):

3285, 3913, 4454, 5082, 5620, 6241, 6780, 7409, 7947, 8575, 9111, 9748, 10283, 10455, 10992, 11621, 12248, 12787, 13414, 13955, 14581, 15208, 15747, 16373, 16923, 17543, 18084, 18708, 19264, 19880, 20442, 21050, 21758, 22210, 22760, 22925, 24090, 24717, 25260, 25888, 26511, 27051, 27677, 28218, 28849, 29389, 30021, 30559, 31186, 31723, 32352, 32889, 33520, 34070, 34232, 34700

5kHz spectra:

6480, 7359, 7651, 7943, 12248, 12540, 12832, 17429, 17721, 18013, 18600, 18892, 19184, 23492, 23784, 24076, 28379, 28671, 28963, 29844, 30136, 30428, 33854, 34733, 35025, 35317, 39625, 39917, 40209, 44806, 45098, 45390, 45982, 46274, 46566, 50871, 51163, 51455, 55756, 56048, 56340, 57224, 57516, 57808, 61231, 62110, 62402, 62694, 67001, 67293, 67585

ADC/TDC corrections

The RTOF ADCs and TDCs suffer from gain differences which add unwanted noise to the spectra and thus must be corrected to obtain a more accurate signal from the raw data. The signal correction algorithm for the histogram and event data utilises a set of re-calibration adjustment values for the 16 ADC (resp. TDC) channels. For each record of events and histogram data, the raw signal is multiplied by the appropriate adjustment value (using the bin number to determine the channel) to obtain the corrected value. These adjustment values (or correction factors) are calculated by summing the contribution in a spectrum of each ADC / TDC individually, and then normalising these sums to obtain a correction factor to apply on each ADC / TDC. The code used for the calculation of the correction factors is given below:

```
// calculate the ADC factors for each spectrum
for (i=3392; i<xThis_PDS_RTOF_DATA_TABLE_L2->records-16; i=i+16)
{
  // calculate the mean ADC values for the 16 ADC
  for (k=0; k<16; k=k+1)
  {
    anADC_mean[k] += xThis_PDS_RTOF_DATA_TABLE_L2->record[i+k].histogram_counts;
  }
```

```
}

// calculate the mean of the 16 mean ADC values previously calculated, to be used for
normalisation
for (k=0; k<16; k=k+1)
{
    anADC_norm += anADC_mean[k]/16;
}

// calculate the correction factor for each ADC
for (k=0; k<16; k=k+1)
{
    anADC_correction[k] = anADC_mean[k]/anADC_norm;
}

// adjust data according to the ADC (histogram counts) correction factors
for (i=0; i<xThis_PDS_RTOF_DATA_TABLE_L2->records; i=i+1)
{
    nCorrectedData = xThis_PDS_RTOF_DATA_TABLE_L2->record[i].histogram_counts /
        anADC_correction[(xThis_PDS_RTOF_DATA_TABLE_L2->record[i].bin - 1) % 16];
    xThis_PDS_RTOF_DATA_TABLE_L2->record[i].histogram_counts = nCorrectedData;
}
```

Below is an example of the ADC/TDC correction technique applied to FM Storage Source data
(histogram / ADC counts), where the raw signal is in black and the spectrum corrected for the
electronic noise + ADC/TDC pattern is in red.
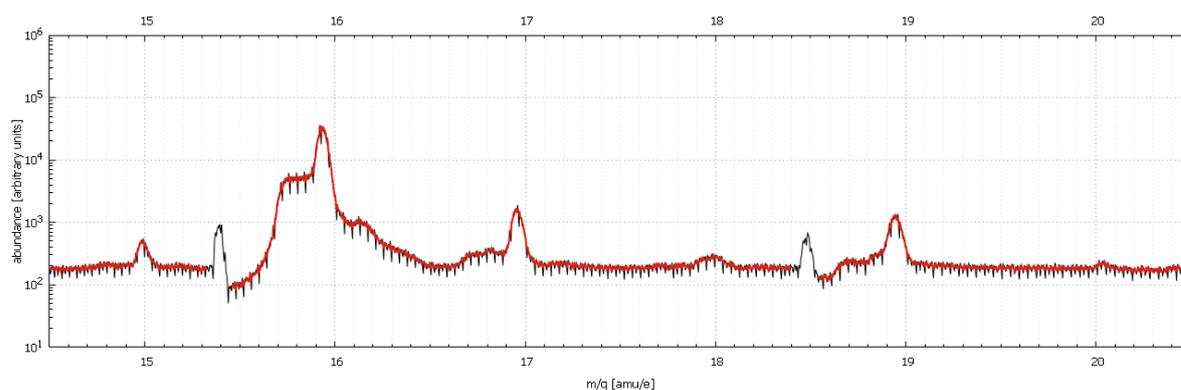
Limiting the data range

The RTOF L2 data files are quite large and contain an excessive number of bins in most cases. In
order to reduce the size of RTOF L3 data files, the limited range of bins to be retained in the L3
data is listed for each mode ID in the PDS RTOF Mode ID table files. This is defined by all bins
occurring between a minimum and maximum bin number (i.e. the bin values of fields
'.retain_bin_start' and '.retain_bin_stop').

4.6. Convert signal to counts (ions) per second

A "signal factor" (as stored in the L3 product RTOF_HK_TABLE) is calculated from the L2 data in order to convert input L2 data into the resultant L3 signal representing counts (ions) per second.

For Storage Source (SS) spectra, the "signal factor" is defined as the inverse of the ratio of total histogram counts (with ADC corrections) to total event counts (with TDC corrections) across the entire spectrum multiplied by the integration time in seconds.

SS_signal_factor = 1 / ((total histogram counts / total event counts) * integration time)

This factor is then multiplied by the ADC corrected L2 histogram data to obtain the resultant signal in counts (ions) per second.

For Orthogonal Source (OS) spectra, only event data is available, so the "signal factor" is simply the inverse of the integration time in seconds.

OS_signal_factor = 1 / (integration time)

This factor is then multiplied by the TDC corrected L2 event data to obtain the resultant signal in counts (ions) per second. Below are examples of the signal calibration to ions per second (blue) from Histogram counts (black) and Event counts (red). Both spectra were measured with a 200-second integration time.
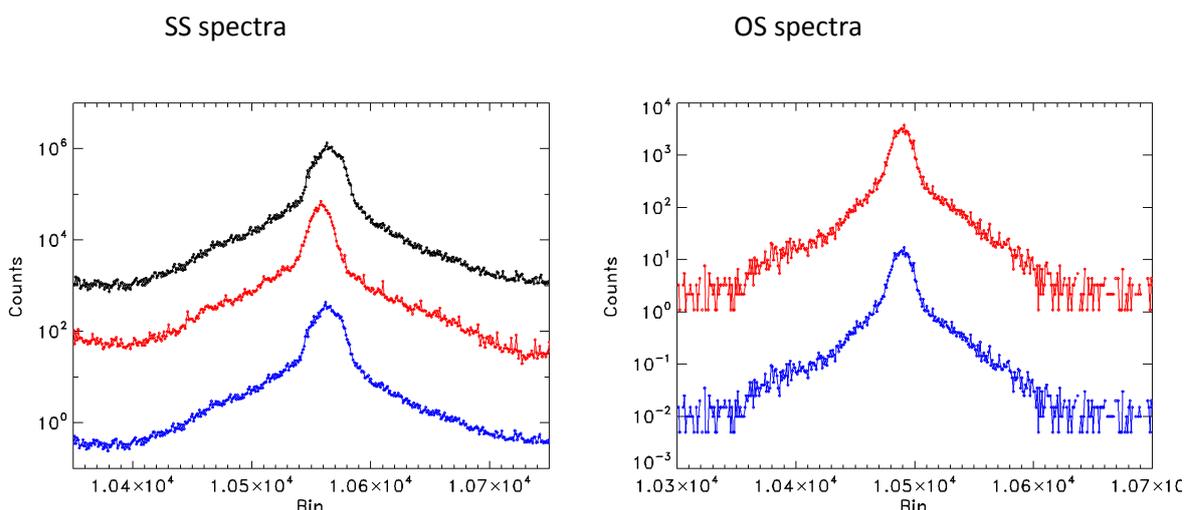
4.7. MASS SCALE CALIBRATION

The mass scale calibration for each spectra is calculated using the factors C and t0 in the equation below.

$$mass \; = \left(\frac{(\text{Time of Flight} - \text{t0})}{\text{C}} \right)^2$$

These factors are derived by matching the known masses of species in the collected gas sample with the location of their peaks in the data. As described in section 1, the location of these mass peaks is expected to be fairly consistent. However their location will depend upon the instrument settings. Thus for each instrument Mode ID there is a RTOF Mass Peak Search Table file (dated for reference) which describes the expected location (in bins) of the peak of several key species expected to be present in the measured sample, i.e. H_2O, CO, and CO_2 for the non-GCU spectra and He, C, CO, CO_2, and 84Kr for the GCU spectra. A bin "window" is defined where this peak alone is meant to be located, allowing for slight fluctuations in the peak locations.

Each spectra locates the most appropriate RTOF Mass Peak Search Table file, i.e. the most recently produced file with the same listed Mode ID via a subroutine. All mass peaks listed in this RTOF Mass Peak Search Table file are sent through the Peak Finder (see below) and then used as needed to determine the factors C and t0 as well as the resultant mass scale precision (from the average PPM deviance).

Peak Finding / Fitting

Mass peaks are first located in the corrected L3 data within their "bin search window" (from the RTOF Mass Peak Search table) by a simple peak finder. Found peaks are then fit to a simple Gaussian to produce a more accurate determination of the peak centre (which is then related to the known mass).

The peak finder first locates the bin with the maximum signal within the "bin search window" of the desired peak and this value is adopted as the potential peak height (amplitude). A minimum height threshold is set to 2 times the L3 signal factor. If this potential peak height is greater than the minimum height threshold and four or more bins contain signals within 50% of this potential peak height then the peak is considered to be found. If not enough peaks are within 50% of the potential peak height then the bin with the next greatest signal is considered as the potential peak height. This process is repeated until the criteria is either met or the potential maximum signal is lower than the minimum height threshold. If the criteria is met then the peak height is set to the mean signal amplitude of the bins within 50% of the potential peak height and the peak centre is set to the mean of the bin numbers that meet the same criteria. Otherwise these values are all set to zero.

For peaks found with the simple peak finder, the Marquardt non-linear curve fitting algorithm is used to fit the peaks (as described in P.R. Bevington, "Data Reduction and Error Analysis for the

Physical Sciences," McGraw-Hill, 1969). The expected peak shape is a pseudo-Voigt form; however a simple Gaussian is used as the proxy-fitting shape since the Gaussian portion of the peak shape comprises the majority of the signal. The peak centre and height from the simple peak finder are used as initial estimates for the Gaussian function's centre and amplitude. Additionally the initial estimate of the Gaussian function's width is set to 100 (found to be the most reliable in achieving valid results from the curvefit algorithm). Data points with signals equal to or greater than 2% of the initial estimated peak height are given equal weighting (equal to 1). Data points with signal below this threshold are given much smaller weights (10^{-4}) as the wider Lorentzian portion of the pseudo-Voigt peak shape becomes significant at that point and will skew the results of fitting to a simple Gaussian.

The results of curvefit are tested to ensure their validity by checking against the following criteria:

- The returned Gaussian function's height is within 0.25 and 4 times the initial estimated peak height.
- The returned Gaussian function's centre is within the "bin search window".

If the following requirements are met then the peak's entry in the L3 spectra file's RTOF Mass Calibration table will reflect the curvefit results. If the curvefit results do not meet the criteria then the peak's entry in the RTOF Mass Calibration table will instead reflect the results from the simple peak finder. The peak centres determined are then used as the peak locations (proxy for time-of-flight) to match them with a known mass in the calibration process.

Below are two examples of the results from the peak finding and fitting process. The edges of the "bin search window" are marked by vertical blue dashed lines, the peak centre and amplitude found by the simple peak finder is shown by a red X, and the fitted peak is shown by a thick red line.

Found Peak with Successful Curvefit
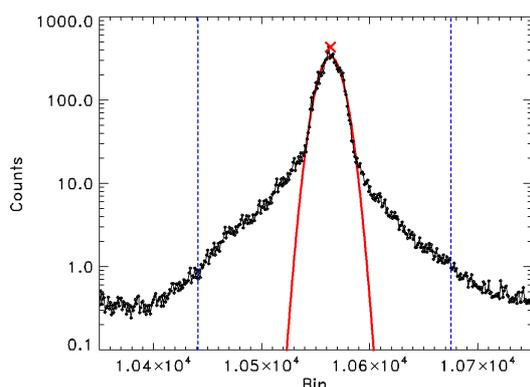
Found Peak with Unsuccessful Curvefit
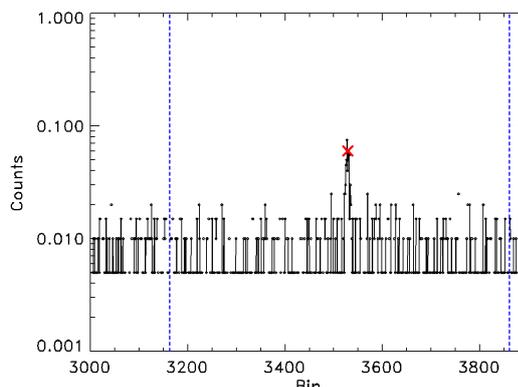
Calibration/Verification peaks

The mass peaks listed in the "Mass Peak Search Table" files for mass scale calibration fall into two categories: 'calibration' peaks, and 'verification' peaks. 'Calibration' peaks are used to determine the calibration factors C and t0. Therefore these mass peaks should only be the most prominent and reliable for the specific Mode. 'Verification' peaks are then used along with the 'calibration' peaks, to determine the average PPM deviance of all known peaks to the mass scale assumed by the factors C and t0.

GCU-aided calibration

As mentioned above, GCU measurements have an advantage in accurate mass-scale calibrations as the measured signal represents a known gas mixture with sufficient amplitude peaks that cover a wide mass range. In order to take advantage of these GCU measurements, all non-GCU modes have an accompanying GCU mode such that the mass peaks can be expected in the same locations (and thus C and t0 will ideally be the same). The GCU companion Mode ID is found from the supplied PDS RTOF Mode ID table file.

After performing self-calibration of C and t0, non-GCU spectra will then locate the most recent L3 GCU spectra file through a subroutine, and load its values for the mass calibration factors C and t0. The PPM accuracy of all the found 'verification' mass peaks of the non-GCU spectra are calculated using the C and t0 of the most recent L3 GCU spectra file. If the average PPM deviance of all 'verification' mass peaks using the GCU-reference C and t0 is greater than a given threshold (current standard is 500 ppm) then the self-calibrated values will be adopted to calculate the mass scale. Otherwise the GCU-reference values will be adopted. Additionally, a flag may be set in the software to force the GCU values to be used (logged in the field "ROSINA_RTOF_SCI_ALLOW_NONGCU_CAL" in the RTOF_HK_TABLE). This information is logged appropriately in the RTOF_HK_TABLE where the "GCU_*" and "SELF_*" values are labelled with "OFF" or "ON" status as appropriate.

Mass Scale Precision

The mass scale precision has been fixed to a value of 0.005 u/e due to the known uncertainty of the instrument.

Choosing the Mass-Scale and Data Quality

GCU spectra will by default always use their self-calibrated mass scale. Non-GCU spectra will adopt the mass scale of their reference GCU spectra so long as the average PPM deviance of the verification peaks is less than 500 ppm when using the GCU mass calibration factors. Non-GCU spectra which do not meet this threshold will adopt their self-calibrated mass scale instead.

The data quality ID is determined from the decision to use non-GCU mass scale in favour of the (reference) GCU mass scale, the average PPM deviance of the adopted mass scale, the spectra

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background level, and the number of peaks from the Mass Peak Search Table that were found/fit during processing. Spectra whose average PPM deviance is less than 500 when using the reference GCU mass scale are assigned a data quality ID of "0" which is the highest quality. Non-GCU spectra which adopt self-calibrated mass scales with an average PPM deviance of less than 500 ppm are assigned a data quality ID of "1" (GCU spectra cannot have this data quality ID as their GCU and self-calibrated mass scales are the same). When a spectra's adopted mass scale has an average PPM deviance greater than 500 ppm, the data quality ID of "2" is assigned. Spectra with a background signal level (average signal within the background determination region specified in the Mode ID table) that is greater than a set "enhanced noise threshold" (currently 0.5 ions/s) have a data quality ID set to "3". If less than two peaks from the Mass Peak Search Table could be found/fit then mass scale calibration/verification cannot be performed and the data quality ID is set to "4". If only two peaks from the Mass Peak Search Table could be found/fit then the data quality ID is set to "5".

Below is the list of data quality IDs and their descriptions, as listed in the L3 PDS Header.

0 means 'Nominal quality, avg. PPM deviance < 500'
1 means 'Self-calibrated, GCU avg. PPM deviance >= 500, SELF < 500'
2 means 'Adopted mass scale avg. PPM deviance >= 500'
3 means 'Enhanced Noise'
4 means 'Not enough peaks found for accurate calibration/verification'
5 means 'Self-calibrated from only two peaks, uncertain PPM deviance'

NOTE - If the background signal is greater than the "enhanced noise threshold", then the data quality will be set to 3 regardless of the applicability of any other data quality levels (e.g. not enough peaks were found, self-calibrated, etc.).

4.8. Density of species j

Fragmentation
- Molecules are dissociated/ionised by electron impact.
- Fragmentation pattern depends on electron energy.
- Fragmentation patterns are instrument dependent. It is not correct to take patterns for example from the NIST without being aware of the uncertainties attached to this!
- For RTOF the nominal electron energy is 70 eV.
- The fragmentation tables in the archive contain the parent and all non-zero daughters.
- The numbers are normalized to the highest peak (100%) which is not necessarily the parent (analog to the NIST tables).

Ionisation cross sections for different species can be found in literature, but be aware of the uncertainties!

Literature on ionisation cross section shows large variability in the results, e.g.
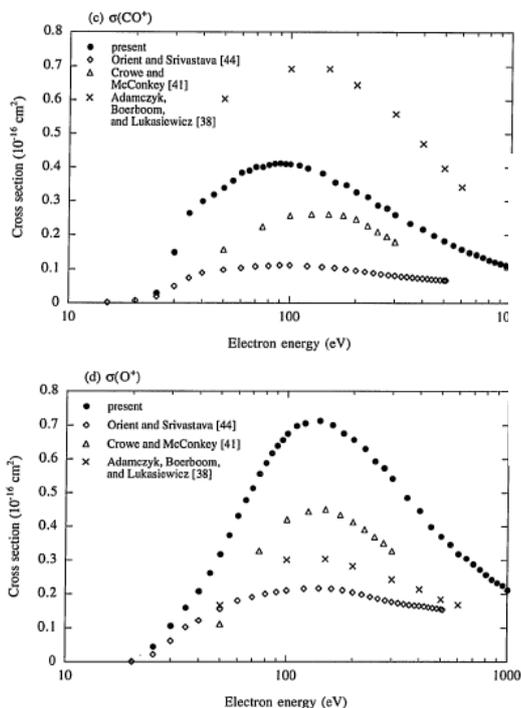
Fig. h: Different Ionisation cross sections for CO2 into CO^+ and O^+ from the PhD thesis of HC Straub.

Sensitivity:

$$S = Cs(I_e) * tau * yield$$

With

Cs(I_e): cross section (function of electron current, electron energy and species)
tau: transfer function (function of energy and resolution)
yield: detector yield relative to N2, 3000V (function of energy and species)

Sensitivities for calibrated compounds can be found in the archive.

Calculating densities

c)   From fragments

$$I_i (\mu A) = I_e (\mu A) \, S_j (cm^3) \, Q_{ij} \, n_j (cm^{-3})$$

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Ie: electron current
Sj: Sensitivity for gas j
Qij :   Fragmentation pattern for ion species i of gas j e.g. O^+ from CO^2
n_j: density in cm^{-3} for species j

d) From the parent species

$$I_{main} (\mu A) = I_e(\mu A) \; S_{parent} \; (cm^3) \; n(cm^{-3})$$

S_{parent} Sensitivity for parent species (can be found in the archive or approximated from literature and the energy dependence of the instrument's mass-dependent sensitivity (see above).

4.9. Using COPS data for the absolute calibration

As described above, detector ageing of the MCP plays a major role. While relative gain between pixels was measured regularly throughout the mission (pixel gain files in the archive) and the relative overall gain between gain steps could be assessed after the mission by looking at the fragmentation pattern of water, which is supposed to stay constant, the absolute overall gain cannot be measured in flight. However, this can be overcome by using COPS data for calibration, as it measures absolute densities. For a description on how to calibrate RTOF data with COPS see chapter 5.7.

4.10.   Pitfalls, irregularities

High resolution mass spectrometry is an "art" and RTOF was a very complex instrument. There are many pitfalls, some of which are mentioned below:

- The RTOF FS showed a lot of anomalies in flight, starting in fall 2004. Subsequent investigations in March 2005 revealed a break-down of the 9kV power supply. After this time, the highest possible voltage which could be achieved was -2900V. However, at that voltage there was an excessive current of 60 mA on the 24V. The situation of the instrument was not stable. A bake-out of RTOF over a long time (during the Earth flyby in 2007, with RTOF in standby) did not solve the problem. Finally, a fix for the problem was designed by the electronics engineer of UoB and this fix was implemented in spring 2010. The fix consisted of a DPU-controlled procedure to switch repeatedly between the 24V and the 9 kV HV power converters, which resulted in a much lower output voltage than the original 9 kV. One of the voltages in RTOF which could be regulated to 8 kV

(SS_SL, OS_SL or HML) had to be used to regulate this output voltage. All other voltages were deduced from this. In order to be stable, they have to be lower than the regulation voltage. The DPU uses a fixed "on"-time, which is a table value, and then changes the "Off" time according to the output voltage defined. The "On" time is a multiple of 0.7ms (0 ->0.7 ms, 1->1.4ms...). As of January 2011 the following parameters were used:

- o Drift: -1000V
- o T_off min: 40 ms
- o T_off max: 500 ms
- o T_on: Step 8 (equivalent to 6.3 ms)
- o Stepwidth standard: 1 ms/V
- o Stepwidth switch-on: 10 ms/V
- o Output Voltage: -2000 V

- The mass resolution of RTOF is ~500 at FWHM. This allows for precise mass determination, but not separation of species which are on the same integer mass. The mass peak is located on an average mass according to relative abundances.

- The sensitivity of RTOF is lower than for DFMS. As it also produced large volumes of data, it was therefore only operated when close to the comet.

- In May 2015, the filament in the SS broke. It took a few weeks before RTOF could be switched on again with the redundant filament in the SS.

- Due to the many slews of the S/C, RTOF spectra are affected by contamination from sublimating gas from the S/C. Sudden jumps in intensity can therefore be the outcome of a slew.

- After switching on the instrument, some time is always needed to outgas the filament and to get into thermal equilibrium. Therefore always look at the data in context, not at single spectra.

- Dust impacts affect the mass spectra in RTOF as well as COPS intensities. They can be recognised by sudden increases in the COPS density followed by a slower decrease.

5. COPS

5.1. Applicable documents

Details on the ROSINA-COPS sensor can be found in:

a. Balsiger, H., Altwegg, K., Bochsler, P., Eberhardt, P., Fischer, J., Graf, S., … & Müller, J. (2007). Rosina–Rosetta orbiter spectrometer for ion and neutral analysis. *Space Science Reviews*, *128*(1-4), 745-801.

b. ROSINA User Manual including appendix D3-COPS instrument modes (part of the archive)

Details on the data analysis and uncertainty considerations can be found in:

C-Y Tzou, PhD thesis, Univerity of Bern, 2017
(http://biblio.unibe.ch/download/eldiss/17tzou_cy.pdf)

5.2. Short instrument description

The Comet Pressure Sensor (COPS) consists of two gauges. The first is the "nude gauge" which measures the total density of the cometary gas at the location of the S/C. The second gauge is the "ram gauge" which measures the ram pressure (equivalent to the cometary gas flux). The nude gauge uses filaments to emit electrons and to ionise the gas, while the ram gauge uses cold microtip arrays.

The measurement principle is simple: ionise the gas by electrons impact in a certain value and then measure the ion current. The electron energy used is 90 eV. For the ram gauge, neutrals are first thermally equilibrated by collisions with the wall, before being ionised by cold electrons (90 eV) as well).
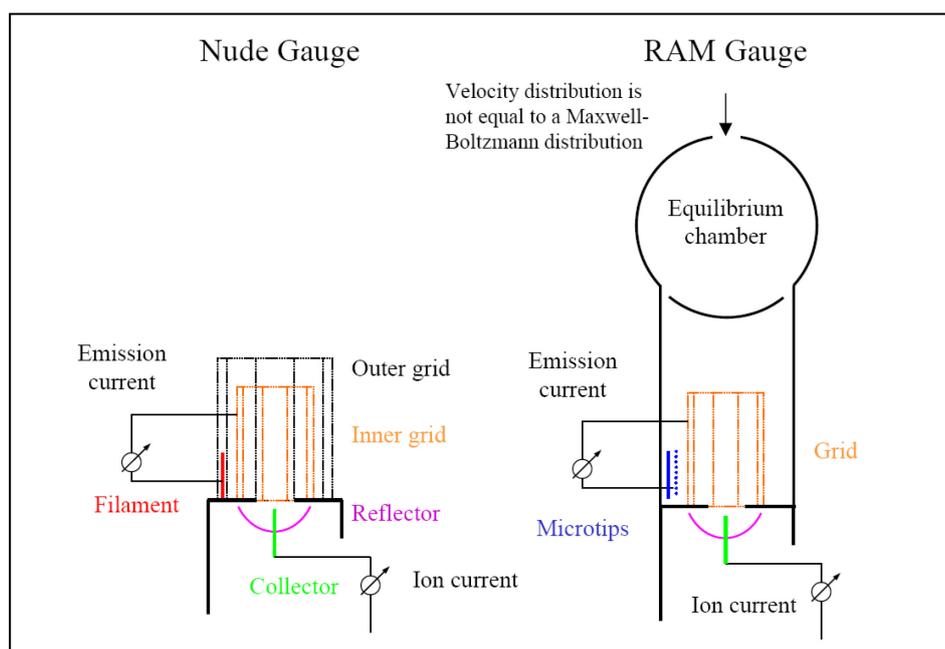
Fig. i: From the two measurements, the expansion velocity can be derived.

The nude gauge

Free electrons emitted from a 17 mm filament at +30 V are accelerated towards a cylindrical anode grid (20 mm diameter, 40 mm height) at150 V. Inside the anode, a thin molybdenum wire (0.15 mm diameter, 38 mm long) collector is mounted and connected to an electrometer. The electrons follow an orbital motion around the collector, ionizing the gas along their path. The measured ion current is directly proportional to the density. The density is measured by an extractor-type gauge (Redhead 1966) which measures lower pressures (no X-ray limit) than a typical Bayard-Alpert gauge and shows better reproducibility. The ion collector is hidden by a shield from the X-rays generated by electrons hitting the anode grid. The created ions are collected with a3-element electrostatic lens-like system (anode-shield-Reflector). The anode (20 mm diameter, 32 mm height) is at 180 V. Such a configuration also prevents solar UV from reaching the collector.

The ram gauge

The gauge is also based on the extractor geometry and has been modified to accommodate a new source of electrons called microtips (see below). The reflector is a hemisphere of 8 mm radius with an apex aperture through which is mounted the collector (0.15 mm diameter, 3 mm long). The anode (16 mm diameter, 19 mm height) is at 180 V. The shield, with an aperture of 3.4 mm diameter at its center, is at 0 V.

The ram gauge boom points toward the comet, while the nude gauge boom is parallel to the solar panels. Half of COPS will never be exposed to the Sun, so half of each boom is sandblasted and the other half is gold-plated. To avoid strong thermal gradients in the ram gauge (it would degrade the measurements) the electronics box is protected by multi-layer insulation.

To calculate the pressure, the DPU used the following formulae:

For the nude gauge:

$$p(mbar)_{NG} = \frac{(Ion\_current_{fil}(A) - Ion\_offset_{fil}(A))}{(Immission\_current_{fil}(A) - Immission\_offset_{fil}(A)) \cdot S_{NG}}$$

For the ram gauge:

$$p(mbar)_{RG} = \frac{(Ion\_current_{mic}(A) - Ion\_offset_{mic}(A))}{(Immission\_current_{mic}(A) - Immission\_offset_{mic}(A)) \cdot S_{RG}}$$

The ion offset value is measured with background mode.
S is the calibration factor, it is about 30 for the nude gauge and 5 for the ram gauge.
This factor depends on the temperature and the ambient gas.
Flux formula for the Ram gauge:

$$phi\_out = 0.25 * \sqrt{\frac{8 \cdot kB \cdot T\_RG}{\pi \cdot mass}} * \frac{p\_RG}{T\_RG * kB}$$

phi_out = gas flux [$1/m^2*s$]

kB = Boltzmann constant = $1.38e^{-23}$ [J/K]

T_RG = ram gauge temp. [K]

mass = 18 amu = $2.9889e^{-26}$ [Kg] (H_2o is the default mass)

p_RG = ram pressure [Pa] = $100*[p(mbar)_{RG}]$

The pressure values given directly in the COPS housekeeping are pressures for N_2 at 20°C. In order to derive the density, this pressure value has to be converted to density as follows:

n (m^{-3}) = p /(kT)   with p in Pa; T=293K, k=$1.380 \cdot 10^{-23}$ J/K

e.g. if p=$1x10^{-10}$ mbar, then n=$2.4x10^{12}$ m^{-3} = $2.4x10^6$ cm^3

5.3. The main operation modes

COPS was either operated in single gauge mode (NG), which means only the nude gauge was operating or in dual gauge mode where both gauges (BG) were operated. This was done due to the limited lifetime of the microtips. It was mostly operated at the highest electron emission, which was 100 µA. However, due to aging of the microtips, the emission current was set to 15 µA later in the mission for the ram gauge. The group of microtips operating at any given time was also changed from 1-3 to 5-8. When the data rate was sufficient, COPS was operated in science mode, which meant that it sent all measured pressure values (1 every 2s), while in housekeeping mode it sent only housekeeping pressures (1 every minute). Each data packet contains 5 minutes of data, which is equivalent to 150 values for each gauge.

5.4. L2, L4 data set description

L2 data is raw data as received from the instrument. They contain some housekeeping, and if applicable, also science data packets (see above). The pressure is calibrated for N2 gas at 20°C and has to be converted to density (see above). For this, one needs the relative abundances of species in the gas. This can be taken from either RTOF or DFMS data. The ionisation cross sections for these species are slightly different and we use 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 from DFMS to compute a weighted average for the ionisation cross section.

L4 data is density data from COPS which has been subjected to this correction procedure and therefore represents actual absolute number density measurements at the position of the S/C. Immediately after switching on COPS, densities measured tend to be higher due to filament outgassing. Normally, it is best to ignore any data taken within half an hour after switch-on, data acquired during slews >5° and the large densities measured late in the mission at close distances to 67P where saturation may have occurred. Additionally, COPS was not always switched-off during WOLs, especially later in the mission. This produced easily noticeable effects, as COPS would react to the WOL with a sharp peak. COPS also

reacts to dust impacts, seen as short-lived (lasting a few minutes) peaks. During enhanced solar activity, COPS also reacts to energetic ions, leading to "noise" in the measured density.

5.5. How to calibrate COPS with MS data

During the development phase of ROSINA, COPS was designed to have similar gas sensitivity to the Granville-Phillips Stabil-Ion Gauge (G.P.) which is a Bayard-Alpert gauge calibrated for N2 with a typical error of 4% - 6% (Granville-Phillips, 2007). Like the G.P., COPS has different sensitivities to different types of gas due to the different individual electron-impact ionisation cross-sections. Therefore, correction factors are needed for pressure/density readouts when measuring gas species other than N2.

One thing to note is that gas density and gas pressure are interchangeable. In the case of COPS, pressure values are given directly in the housekeeping as if measuring only N2 at 20 °C for which the calibration values were obtained in lab. The conversion between density and pressure follows the ideal gas law P = nkT with P being the pressure in pascals, n the number density in m^{-3}, the temperature T = 293 K, and the Boltzmann constant k = 1.38 x 10^{-23} J K^{-1}.

As shown in Equation (3.1), when measuring a non-N2 gas with COPS, the pressure readouts $P_{C;i}$ must be multiplied by a correction factor βi for a single gas species i to retrieve the real pressure of an individual species. The correction/scale factors for individual species used in this study can be found in Table 3.1.

$$P_i = \beta i \times P_{C;I} \qquad (3.1)$$

In space, however, COPS always measured the total pressure/density of the gas mixture in the coma of 67P, not single gas species. Here, we introduce the procedure for deriving the species-dependent correction factor $\beta_{C;total}$ for gas mixtures measured with COPS, as used in Equation (3.2). P_{total} is assumed to be the real pressure for the total gas mixture, and $P_{C;total}$ is the total gas mixture pressure readout from COPS.

$$P_{total} = \beta_{C;total} \times P_{C;total} \qquad (3.2)$$

In Equation (3.3a) $P_{C;total}$ is represented as the sum of the individual species' pressures as seen by COPS. Using the relation between COPS single species pressure and real pressure from Equation (3.1), $P_{C;total}$ can be related to P_i, the partial pressure of individual species i. Partial pressure P_i is expressed with R_i, the volume mixing ratio of species i, in Equation (3.3b).

$$P_{c,total} = \sum P_{c;i} = \sum \frac{P_i}{\beta_i} \qquad (3.3a)$$

$$= \sum \frac{P_{total} \times R_i}{\beta_i} = P_{total} \sum \frac{R_i}{\beta_i} \qquad (3.3b)$$

From Equations (3.2), (3.3a), and (3.3b) we can conclude that the correction factor for mixed gas is as given in Equation (3.4), where r_i is the density ratio of species i to water ($r_i = n_i/n_{H2O}$) and the relation between the volume mixing ratio and the density ratio of individual species relative to water is as shown in Equation (3.5). For in-flight COPS density measurements, the volume mixing ratio or the density ratio of main species relative to water are obtained with ROSINA-DFMS and ROSINA-RTOF.

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$$\beta_{C,total} = \frac{1}{\sum_i \frac{R_i}{\beta_i}} = \frac{\sum_i r_i}{\sum_i \frac{r_i}{\beta_i}}$$

(3.4)

$$R_i = \frac{r_i}{\sum_i r_i}$$

(3.5)

One thing to be noted is that all measurements, including the L4 and L5 datasets, contain both cometary signal as well as spacecraft background. In flight, the background is contributed by the spacecraft contamination (Graf et al., 2008; Schläppi et al., 2010) or the electrometer noise of the instrument itself.

Table 3.1: Correction factors for the pressure measurements of COPS and the Granville-Phillips Stabil-Ion Gauge, extracted from Granville-Phillips (2007).

Gas Species		Scale factor
Helium	He	5.56
Neon	Ne	3.33
Nitrogen	N_2	1.00
Oxygen	O_2	$9.90 \cdot 10^{-1}$
Carbon monoxide	CO	$9.52 \cdot 10^{-1}$
Water	H_2O	$8.93 \cdot 10^{-1}$
Argon	Ar	$7.75 \cdot 10^{-1}$
Carbon dioxide	CO_2	$7.04 \cdot 10^{-1}$
Krypton	Kr	$5.15 \cdot 10^{-1}$
Xenon	Xe	$3.48 \cdot 10^{-1}$

5.6. Iterative calibration of the mass spectrometry data

Once COPS has been calibrated for the relative abundance of the main species, the result can be used for an absolute calibration of the MS data (RTOF and DFMS). The sum of all species has to yield the same total density as was measured by COPS. This is done for L5 data for DFMS and RTOF. For this, the closest MS data for 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 are retrieved from DFMS and H_2O, CO, and CO_2 from RTOF and their relative abundances are applied to COPS data (see above). The closest COPS density (L4) is then used to get an absolute value for the densities of these species for the MS.

5.7. Velocity

Velocity calculation can be done in the BG mode. Details and formulas to be used may be found in

C-Y Tzou, PhD thesis, University of Bern, 2017
(http://biblio.unibe.ch/download/eldiss/17tzou_cy.pdf)

Care has to be taken to remove the background first.

5.8. Pitfalls and irregularities

COPS is a simple instrument which is long-term stable. As such, derived densities in L4 are accurate. However, there are a few things to be considered:

- Densities derived are at the location of COPS. These are not production rates.
  - Because COPS has a large field of view, it also detects small changes happening almost everywhere on the S/C such as slews which expose different areas of the S/C to the Sun.
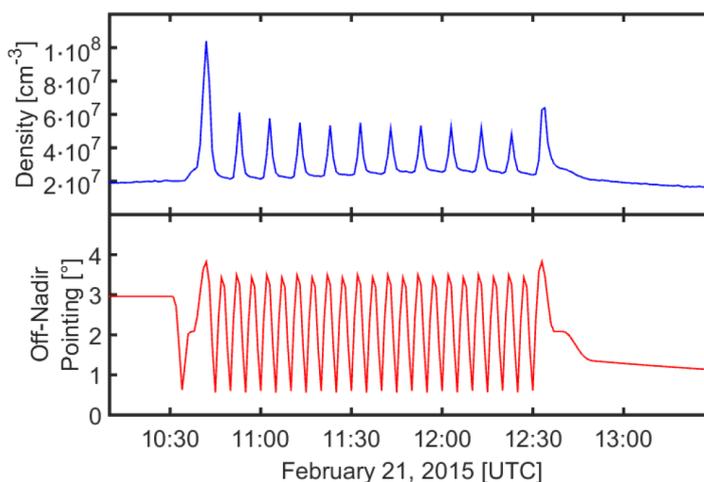
COPS reaction to slews. Off-nadir pointing was between -3° and +3°. At +3° there was always a peak in COPS density due to outgassing of the S/C.

- COPS also detects dust grains impacting directly or close by. This is seen as spikes in the data which have a fast rise and a somewhat slower decrease.
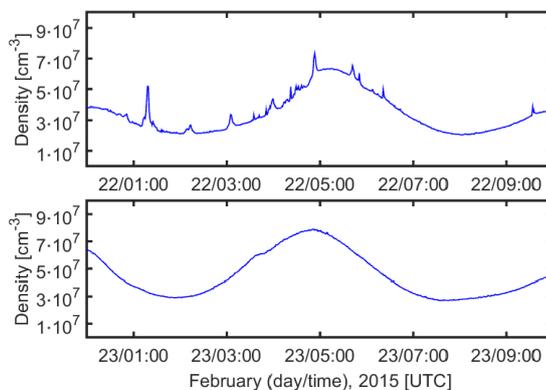
COPS signal with / without dust impacts.

- COPS was also operated during WOLs, clearly characterised in the data by large sharp peaks.
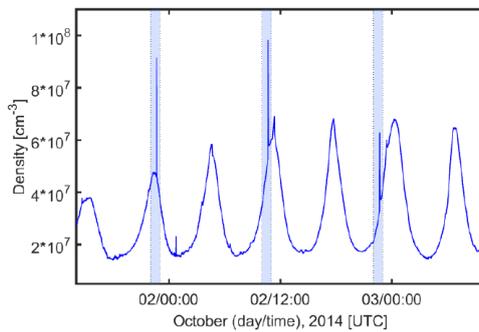
WOL peaks in COPS data (blue shaded areas).

- COPS is adversely affected by exposure to large amounts of high-energy electrons. This manifests as excessive noise.