An automatic pipeline processing software for secondary ion time-of-flight mass spectra of Rosetta/COSIMA

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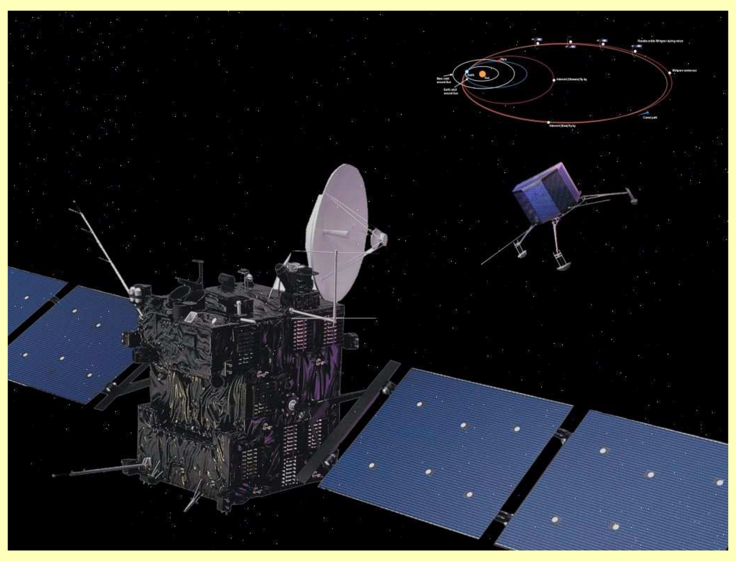

Rosetta spacecraft and lander Philae (graphics ESA)

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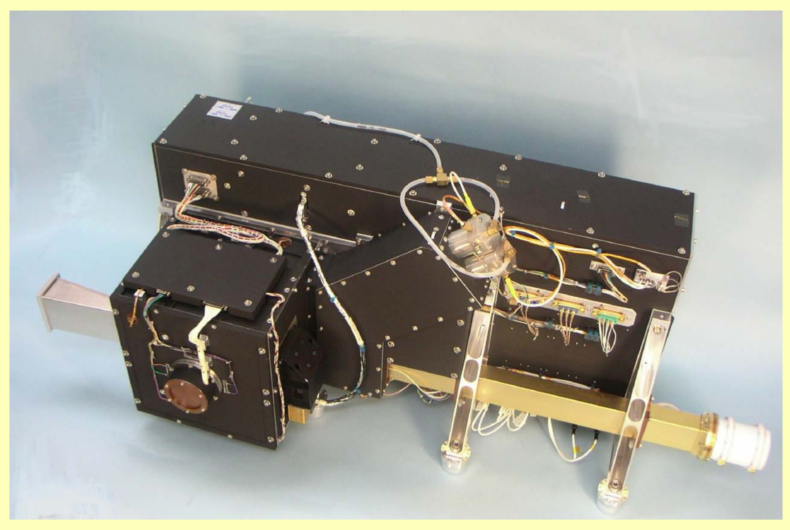

COSIMA instrument in-flight configuration

Abstract

The COmetary Secondary Ion Mass Analyser (COSIMA) on board the Rosetta orbiter will collect and analyse dust grains in the coma of comet 67P/Churyumov-Gerasimenkov beginning in 2014. COSIMA is a high-resolution time-of-flight mass spectrometer ($m/\Delta m \approx 2000$ at $m = 100$ amu; from FWHM; [2]). We expect to obtain thousands of COSIMA mass spectra during the entire Rosetta mission at the comet. In order to be able to handle and efficiently evaluate such a large amount of data, we develop an automatic data processing software. The resulting data is a peak list, giving – for each peak identified in the spectrum – peak intensity, exact mass, suggested ion species, etc. This peak list will serve various purposes: 1) identification of interesting spectra for subsequent more detailed evaluation; 2) input for statistical multivariate analyses (e.g., Corico, Principal Component Analysis [1]); 3) input for further automatic data processing, like, e.g., intensity maps from COSIMA raster scans. We present the current status of our pipeline software and show examples for its application to COSIMA laboratory spectra.

Sample Peak List

```
peaklist.txt        Wed Jun 18 17:39:29 2008        1

RESULTS OF LEVEL 1 PROCESSING
THIS FILE CREATION TIME      = Mi 18 Jun 2008 14:19:21 CEST
TOTAL NUMBER OF COUNTS       = 9638887
MASS CALIBRATION             = 8 lines
MASS CALIBRATION LINES       = H, C, CH3, Na, Si(CH3)3, In, Si2O(CH3)5, Au,
MASS CALIBRATION ERROR       = 1.4758038e-05
MASS CALIBRATION           A = 1586.9969   B =   4064.2398
DEADTIME CORRECTION          = APPLIED
BACKGROUND CORRECTION        = APPLIED

Mass            = Line mass (amu)
Mass_err        = Uncertainty in mass determination (amu)
I_l             = Line intensity (total counts)
I_b             = Average background intensity (per channel) subtracted
I_l/I_tot       = Line intensity/total intensity
LF              = Line deconvolution; s1/s2/d1/d2: two peaks deconvolved; xx: no deconvolution
Ion Species     = Possible ion species and delta m in amu

 Mass #   Mass   Mass_err    I_l    I_b I_l/I_tot LF  Ion Species        delta m      Ion Species       delta m
    1    1.0112   0.0010   74719    92  7.75e-03 s1 1H                0.0039449138
    2    2.0192   0.0011     939    12  9.74e-05 s1 1H2               0.0041418912 2H               0.0056901772
    3    3.0265   0.0010     206    11  2.14e-05 s1 1H3               0.0035807376
    6    6.0272   0.0020     104    11  1.07e-05 s1 6Li                0.012595400
    7    7.0111   0.0036     742    14  7.70e-05 s1 7Li              -0.0043650215
   10   10.0104   0.0019     392    12  4.07e-05 s1 10B              -0.0020274664
   11   11.0069   0.0020    1330    15  1.38e-04 s1 11B              -0.0018561065
   12   11.9983   0.0012   12133    48  1.26e-03 s1 12C              -0.0011736085 24Mg2+           0.0063054415
   13   13.0051   0.0016   10443    43  1.08e-03 s1 12C_1H           -0.0021625987 13C              0.0023075933
   14   14.0147   0.0006   18848    43  1.96e-03 s1 12C_1H2         -0.00036030304
   15   15.0230   0.0017   28625    45  2.97e-03 s1 12C_1H3          7.8521853e-05 14N_1H           0.012654576
   16   16.0209   0.0050     547    15  5.67e-05 xx 14N_1H2           0.0026829917 13C_1H3         -0.0054228703
   17   17.0040   0.0002     198    14  2.06e-05 s1
   18   18.0325   0.0012     279    16  2.90e-05 s1 14N_1H4          -0.0013751865
   19   19.0141   0.0002     448    15  4.65e-05 s1
   20   19.9823   0.0056      48    13  4.97e-06 xx 40Ca_2*           0.0015496413
   23   22.9888   0.0004  645732  1487  6.70e-02 s1 23Na            -0.00037483127
   24   23.9843   0.0024   41477    91  4.30e-03 s1 24Mg            -0.00017966539 48Ca_2*          0.0085952346
   25   24.9883   0.0027   11004    49  1.14e-03 s1 25Mg              0.0029901301 24Mg_1H         -0.0040397799
   26   26.0128   0.0064   17153    70  1.78e-03 xx 12C2_1H2         -0.0022740057 25Mg_1H          0.019714006
   27   26.9794   0.0024   82451   257  8.55e-03 d1 27Al             -0.0016375152 26Mg_1H         -0.010517147
   27   27.0186   0.0033   54932   257  5.70e-03 d2 12C2_1H3         -0.0042844480 26Mg_1H          0.028772576
   28   27.9768   0.0025  352188   665  3.65e-02 s1 28Si             0.00045922510
   29   28.9789   0.0039  102019   268  1.06e-02 s1 29Si              0.0029123899 28Si_1H         -0.0053444521
   29   29.0332   0.0045   35942   268  3.73e-03 s2 12C2_1H5         -0.0054195480 12C_16O_1H       0.030965960
   30   29.9778   0.0025   15915    84  1.65e-03 s1 30Si              0.0045843666 29Si_1H         -0.0059651654
   30   30.0399   0.0055    2246    84  2.33e-04 s2
   31   30.9937   0.0070   11703    78  1.21e-03 xx 30Si_1H            0.012633951 31P              0.020467693
   32   31.9980   0.0029     373    40  3.87e-05 s1 32S                0.026438805
   33   32.9893   0.0042     121    41  1.26e-05 s1
```

Figure 4: Sample peak list generated from a COSIMA spectrum.

Future Improvements

- Extensive testing required!
- Peak profiles of TOF-SIMS instruments are well-known for being non-Gaussian shaped. Peak fitting with a "standard" profile derived from the spectrum itself (e.g., lines used in Figure 2) will be tested.
- Deconvolution of unresolved double peaks.
- Assignment of ion species: consider isotopic ratios, potential hydride contributions, organic compounds, etc. to improve peak assignment [3].
- Improve removal of instrumental artefacts (e.g., non-linearity correction for TDC, improved background determination).

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Overview

- After Rosetta's arrival at comet 67P/C-G in 2014, COSIMA will produce thousands of mass spectra.
- Automatic data processing will be required to manage this large amount of data (Figure 1).
- Mass calibration, dead time correction, background removal and removal of instrumental artefacts can be performed automatically.
- Single and double peaks can be identified from $\mathrm{FWHM}/\sqrt{(m)}$ (m being the peak mass) obtained from a Gaussian fitted to the peak profile (Figure 2).
- Deconvolution of double peaks is rather straighforward for resolved double peaks (Figure 3).
- Peak lists are generated, containing exact mass, line intensities, etc. (Figure 4).
- Peak list serves as quick-look data and as input for higher level data processing, e.g., maps (Figure 5) or multivariate statistical techniques [1].

Flow Chart

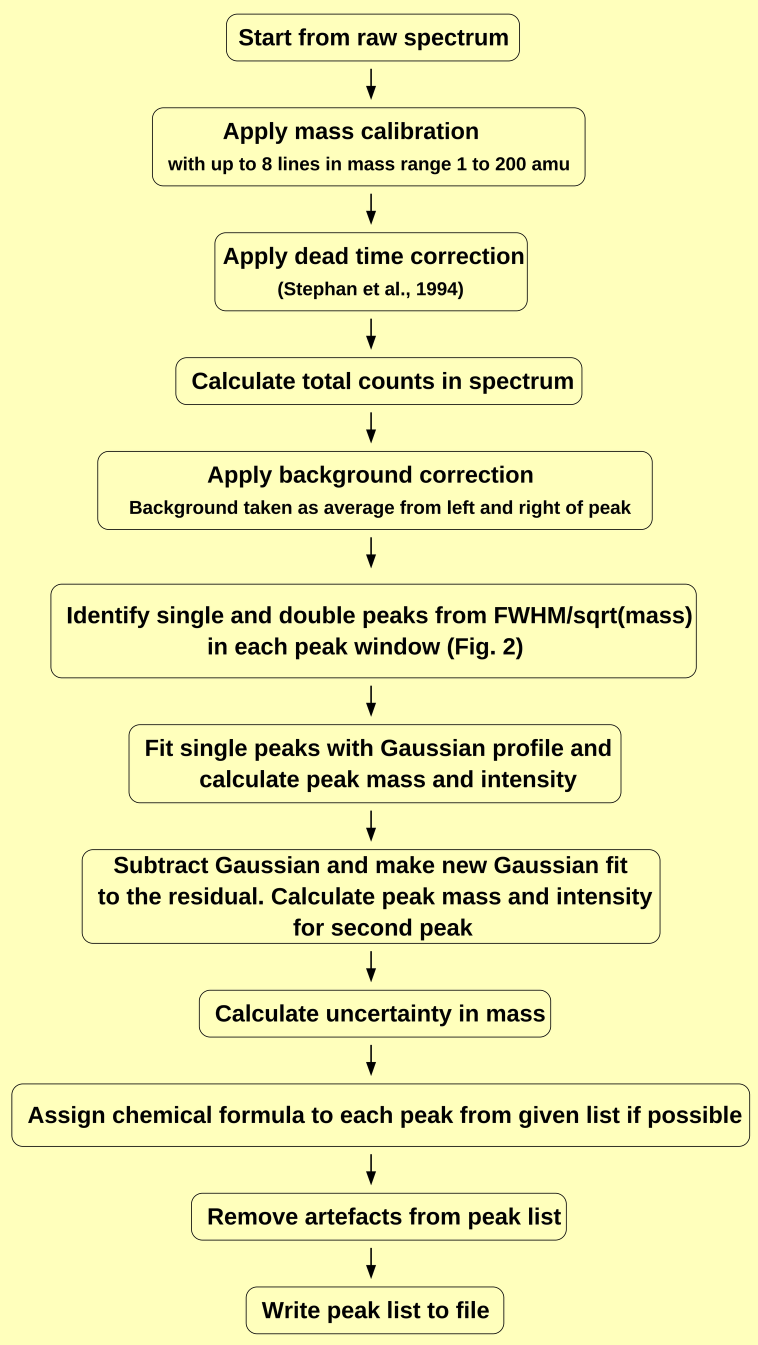

Figure 1: Simplified flow chart for COSIMA spectra processing.

References

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COSIMA Peak Width

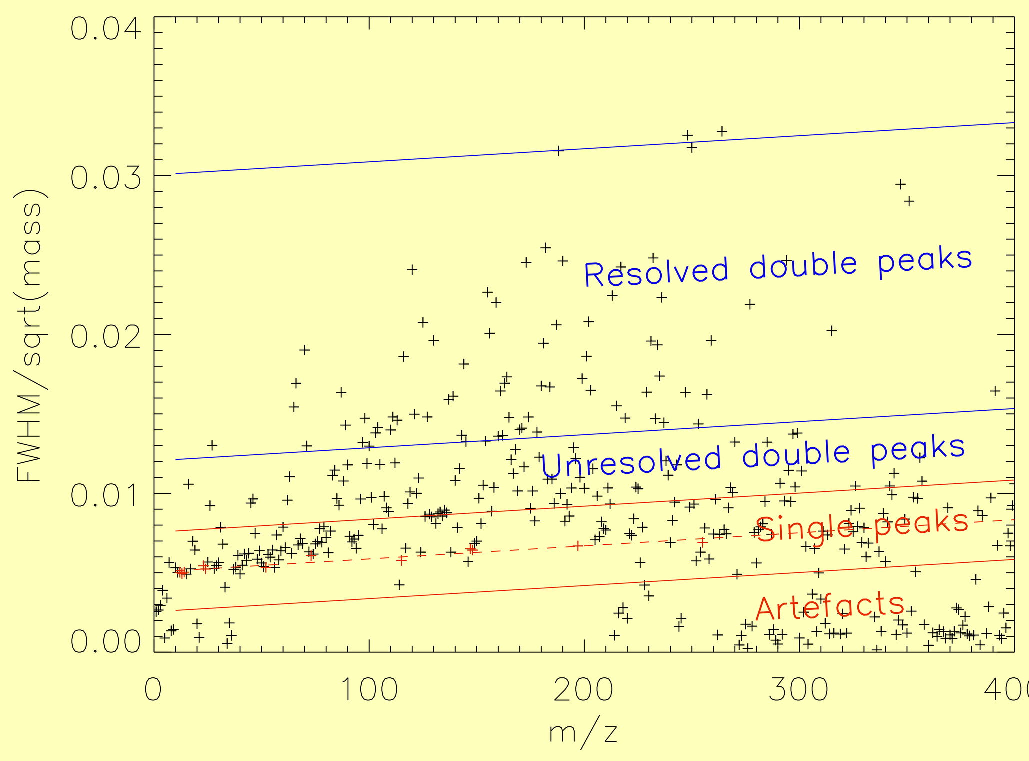

Figure 2: The $\mathrm{FWHM}/\sqrt{m}$ from fitting a Gaussian curve to peaks in the mass range 1 to 400 amu is used to identify single and double peaks in the COSIMA spectra. The reference line for single peaks (dashed red line) is defined by a list of 'standard' peaks: masses 12, 13, 14, 23, 24, 52, 73, 115, 147, 148, 197, 255 amu (positive ion mode); 1, 13, 16, 17, 25, 35, 37, 163, 197 amu (negative ion mode).

Peak Fitting

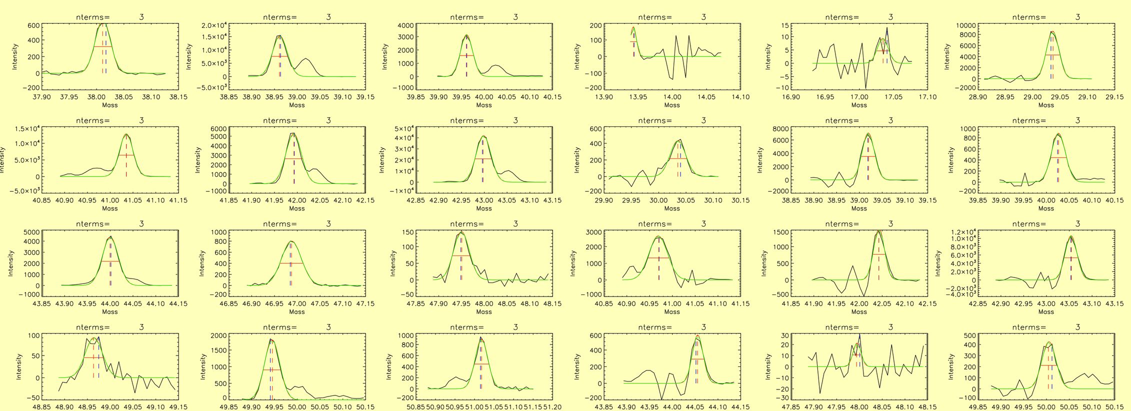

Figure 3: Examples of peaks fitting. *Left three columns:* Single peaks and clearly resolved double peaks with Gaussian fitted to the stronger component. *Right three columns:* Residual lines after removal of the stronger component of the double peak and Gaussian fitted to the residual.

COSIMA Raster Maps

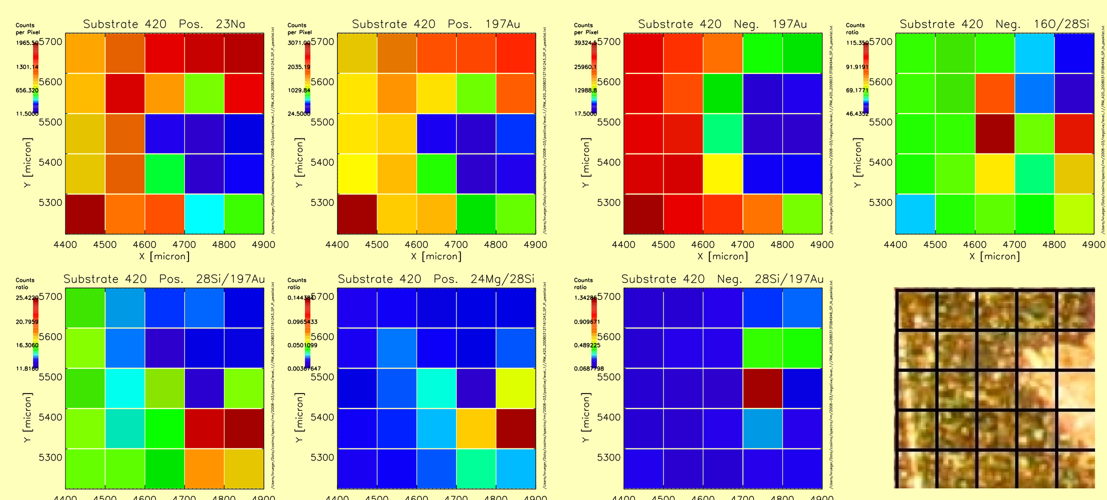

Figure 5: COSIMA raster maps generated from peak lists (in colour) and an optical image (*bottom right panel*). The measurements were taken on synthetic forsterite (Mg_2SiO_4) prepared on a blank gold substrate. *Left two columns:* Positive ion mode; Intensities of ^{23}Na and ^{197}Au, intensity ratios $^{28}\mathrm{Si}/^{197}\mathrm{Au}$, and $^{24}\mathrm{Mg}/^{28}\mathrm{Si}$. *Third column and top right panel:* Negative ion mode; Intensities of ^{197}Au and intensity ratios $^{16}\mathrm{O}/^{28}\mathrm{Si}$ and $^{28}\mathrm{Si}/^{197}\mathrm{Au}$. High intensities or intensity ratios are shown in red while low values are shown in blue. In the intensity ratios the sample is easily identified as the location with the highest ratio, while in the intensity maps the highest signal comes from the gold substrate.