



Sensitivity and fragmentation calibration of the time-of-flight mass spectrometer RTOF on board ESA's Rosetta mission



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ABSTRACT

The European Space Agency's Rosetta spacecraft, with the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) onboard, has been following and observing comet 67P/Churyumov-Gerasimenko since summer 2014. Prior to this period, and due to a technical failure also during this period, optimization and calibration campaigns have been conducted on ground with the Reflectron-type Time Of Flight (RTOF) mass spectrometer as a preparatory work for the analysis of data recorded during the science phase of the mission.

In this work, we show the evolution of the performance of RTOF, and demonstrate and quantify the sensitivity and functionality of RTOF onboard Rosetta. We also present a fragmentation and sensitivity database for the most abundant molecules observed around the comet such as H₂O, CO, CO₂, as well as the noble gases.

1. Introduction

The thorough study of comet 67P/Churyumov-Gerasimenko (67P/C-G) by the European Space Agency's Rosetta spacecraft began in August 2014 as the probe arrived within 150 km from the nucleus. Since then, Rosetta followed 67P/C-G as it reached its perihelion and beyond, providing new insights about comets and how they are formed.

Among the 11 instruments carried by the orbiter, the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) has been designed to analyse the composition of the volatiles in the cometary atmosphere at the location of the Rosetta spacecraft. The science goals of ROSINA are to determine the global molecular, elemental, and isotopic composition of the cometary volatiles in the coma, and to investigate the temporal changes of the comet on its journey around the Sun. Furthermore, ROSINA aims as well to investigate the relationship between cometary and interstellar material and the implications for theories on the origin of the Solar System (Balsiger et al., 2007).

To achieve these goals, a three-sensor approach has been adopted: ROSINA consists of two mass spectrometers, the Reflectron-type Time Of Flight mass spectrometer (RTOF) and the Double Focusing Mass Spectrometer (DFMS), and a pressure sensor, the COmetary Pressure

Sensor (COPS). With a total mass of 34.8 kg, ROSINA represents a little more than 20% of the Rosetta orbiter's scientific payload. Complementing each other to be able to reach the scientific objectives, they also provide the necessary redundancy, due to the long mission duration. The unprecedented discoveries of ROSINA illustrate the importance of in situ measurements in space research (Altwegg et al., 2015; Rubin et al., 2015; Hässig et al., 2015; Bieler et al., 2015). Particularly, the study of the main compounds of the coma – such as H₂O, CO and CO₂ – from ground is highly limited due to near infrared absorption of the Earth's atmosphere (H₂O) or the small permanent electric dipole moments of the symmetric molecules (CO and CO₂) (Mumma and Charnley, 2011; Mall et al., 2016).

The primary goal of RTOF is to identify the species present in 67P/C-G's atmosphere and to investigate their temporal variation. To deconvolve a mass spectrum that results from a gas mixture, it is necessary to know the specific response of the mass spectrometer to each molecule. This response depends on the species dependent sensitivity of the instrument and the fragmentation of molecules inside the ion source. It is therefore necessary to perform an instrument-specific calibration, for as many species expected in the vicinity of the comet as possible. This paper presents the current capabilities of RTOF,

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reduced after two technical failures which occurred in flight, and describes the calibration procedure followed to characterize RTOF, as a preparatory work for the data interpretation.

2. Materials and methods

2.1. Time-of-flight mass spectrometry

Compared with other types of mass spectrometry, time-of-flight (TOF) mass spectrometry has the advantage of being able to record all gas species simultaneously, with a high mass range together with a high temporal resolution. TOF mass spectrometers are therefore natural candidates for the in situ study of volatiles and organic compounds in the vicinity of a comet like 67P/C-G.

The principle of a TOF mass spectrometer is to ionize the gas to be analysed, to accelerate the created ions with the same energy qU so that their speed v would only depend on their mass per charge m/q (Eq. (1)), and to measure the time $t = d/v$ they need to travel through the instrument before they are detected (Eq. (2)):

$$qU = \frac{1}{2}mv^2 \quad (1)$$

$$t = d \cdot \sqrt{\frac{m}{2qU}} \quad (2)$$

Starting from Eq. (2), one can derive Eq. (3) linking the mass to the time of flight of the ions:

$$\frac{m}{q} = \left(\frac{t - t_0}{C} \right)^2 \quad (3)$$

where C and t_0 are constant parameters whose computation will be detailed in Section 2.8.1.

The ionization takes place in an ion source and is usually performed through electron impact: a filament is heated and emits electrons, which are then accelerated into the ionization zone with an energy of $qU_e = 70$ eV. The majority of ionization cross sections for organic molecules have their maxima in this energy range (Mark, 1982). The newly created ions are extracted towards a drift tube by a high-voltage pulse with a duration of typically a few μ s and at a frequency of typically a few kHz, which varies depending on the mass range to be reached: at high extraction frequencies, the heavy ions do not have enough time to fly through the instrument before a new extraction occurs. A detector located at the end of the drift tube measures the arrival time of the ions, from which we can deduce the flight time t of the ions.

The ions formed in the ion source have an initial kinetic energy distribution. Ions with the same mass may therefore not have the same speed and arrive at different times, decreasing the mass resolution of the instrument – the mass resolution being defined as $m/\Delta m$, where Δm is the full width of the peak measured at 50% of the peak height. A good way to lessen this phenomenon was first proposed by Mamyrin et al. (1973): an ion mirror (reflectron) makes the ions turn around at the end of the drift tube and focuses them in a time-focus plane on the detector (see Fig. 1). The first advantage of using an ion mirror is the compensation of the energy dispersion: faster ions penetrate deeper

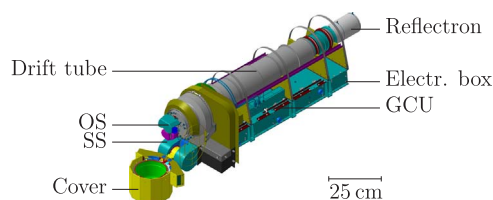


Fig. 2. 3D drawing of RTOF. Aboard Rosetta, the drift tube, the reflectron, and the electronic box – the elongated structure below the ion optical system – remain inside the spacecraft, only the cover and the entrances of the SS and of the OS remain outside.

into the ion mirror and hence have a longer way such that they arrive at the detector at the same time as the slow ones. Secondly, the flight path is also doubled, increasing the mass resolution of TOF mass spectrometers equipped with an ion mirror. Finally, the ion mirror can be designed to also geometrically focus the ions onto the detector to maximize the ion-optical transmission (Scherer et al., 2006). RTOF belongs to this category of reflectron-type TOF mass spectrometers.

2.2. RTOF

RTOF contains two ion sources (see Fig. 2): the Storage Source (SS) and the Orthogonal Source (OS). Both are capable of measuring cometary neutral gas while the latter also allows measuring cometary ions. They can be operated independently or together to study neutrals and ions simultaneously.

Each ion source consists of two filaments, two repellers, a backplane, an extraction grid, two acceleration electrodes and a lens electrode. Additionally, the OS has two entrance lenses to focus the entering ions before their extraction in the source. Sectional views of the sources (based on Balsiger et al., 2007) are shown in Fig. 3 (SS) and Fig. 4 (OS).

In the SS, between two subsequent extraction pulses, the ions are stored between the backplane of the source and the extraction grid where the extraction pulse is applied (see Abplanalp et al., 2010). With this ion storage, it is possible to detect a large fraction of the ions constantly produced in the ionizing portion of the SS, thus effectively reducing the duty cycle.

The drift tube is 83 cm long, giving an effective flight path between the ion source and the detector of 2.2 m thanks to the reflectron. In the present configuration, the ions have a typical energy of 1 keV during their flight.

In its original design, RTOF had a mass resolution larger than 5000 at 50% peak height, and the ability to detect ions up to 2000 u/e (Scherer et al., 2006; Balsiger et al., 2007). However, after a successful in-flight switch on of RTOF during the commissioning phase in 2004, a failure in the main 9 kV high voltage converter occurred, due to outgassing in the nearby potting. This outgassing led to partial discharges along some of the potted cables. It took several years of operation with the laboratory model of RTOF until this failure could be reproduced on ground, and after long investigations and numerous tests with the ground instrument, a software solution was implemented which made possible to operate both the laboratory and the flight models of RTOF the exact same way but at significantly lower voltages

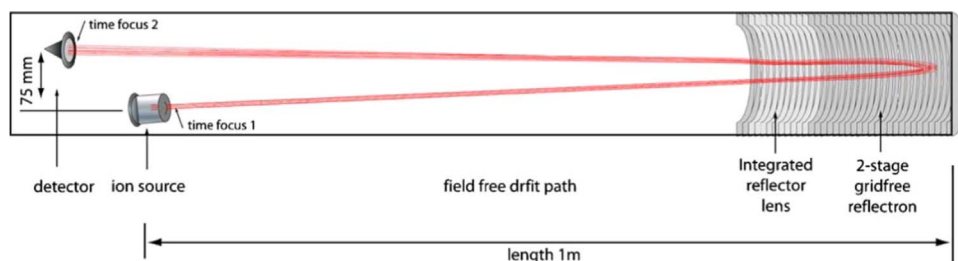


Fig. 1. Principle of a TOF mass spectrometer equipped with an ion mirror (picture based on Scherer et al., 2006).

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