Semi-Volatiles in a Comet (SeVoCo)

Context

Comets are considered to be the most pristine bodies in our solar system. The study of comets can therefore provide information on the chemical composition of the protoplanetary disk (4.6 billion years ago) and on the role of comets in the evolution of Earth and the solar system.

BIRA-IASB contributed to build the ROSINA instrument (Rosetta Orbiter Spectrometer for Ion and Neutral Analysis) designed to measure the gas composition of 67P. Due to its high mass resolution, ROSINA's Double Focusing Mass Spectrometer (DFMS) could measure the coma composition in unprecedented detail and this led to the discovery of a zoo of molecules in the coma of 67P. A wealth of new insights regarding the comet itself, its formation and the early history of our Solar System, was obtained mainly by the study of the volatile species.

SeVoCo addresses a well-hidden type of coma constituents: the semi-volatile species. None of Rosetta's instruments were equipped to measure these types of compounds directly, and only ROSINA/DFMS measurements may possibly provide indirect information on these species. As their name suggests, the volatility of these species is lower than these of the major coma volatile species H_2O, CO and CO_2 and semi-volatile species are characterized by a delayed release from the comet and/or dust as a function of distance from the comet (this is also referred to as a distributed source).

Objectives

The SeVoCo project aims to learn more on semi-volatile species in the coma by evaluating if distributed sources exist for species in the coma.

Methodology

Several effects (instrumental or other) which have a negligible impact on the abundant volatile species (e.g. H_2O, CO_2, CO, O_2) can severely complicate the correct determination of low abundant species. Because semi-volatile species are expected to have a low abundance, a large part of the project involved the improvement of DFMS mass calibration. An accurate mass calibration is needed for the correct identification of species in a mass spectrum and is essential to allow the creation of sum spectra. Sum spectra are an invaluable tool for the detection and identification of minor species, be it semi-volatile species or other. By using sum spectra, the total uncertainty on the results is reduced and species with an abundance very close to the noise level which are not apparent at the single-spectrum level can be highlighted.

Results

As a first step, during the SeVoCo project semi-automatic routines were developed to identify and address (correction/removal) spectra with data issues. This clean dataset was used to investigate Cl, HCl and the $^{37}Cl/^{35}Cl$ isotopic ratio in the coma for the complete mission at the single spectrum level.

The overall $^{37}Cl/^{35}Cl$ isotope ratio for the coma was found to be 0.336 ± 0.017 and its corresponding $\delta^{37}Cl$ value of 51 ± 55 and is in agreement with the isotopic ratio from Earth and most other Solar system bodies. Because there was more Cl found than can be explained by only HCl and NH_4Cl as neutral species in the coma, an additional source for Cl needs to be present in the coma. Cl from this additional source is not readily released from the nucleus and/or dust grains and points to a distributed or semi-volatile source. Unfortunately, the identity of the semi-volatile chlorine-bearing source could not be established.

Secondly, a model was developed for the accurate mass calibration of spectra with a nominal mass between 13 and 69 for the complete mission to allow the creation of sum spectra. It was found that although DFMS is provided with a feedback loop to remove temperature effects in the instrument, it was found that remaining temperature and thermomechanical effects play an important role in mass calibration. The new model allows to accurately align spectra (to better than 1 detector pixel) and enables the creation of sum spectra.

Some of the lowly abundant species detected by DFMS can be linked to refractory elements (Si, Na or Fe). Si, for example is enhanced relative to common volatiles during off-pointing events which indicates a much more uniform and extended distribution of atomic Si in the coma, possibly associated with a distributed source. The question remains how exactly these refractory atoms end up in the gas phase and further studies are required to approach a credible answer.

Conclusions and recommendations

During the SeVoCo project, Cl and refractory species have been found to show a distributed source. The term “semi-volatile” may not have been the optimal name for the group of all species that can be defined as having a distributed source here as it inherently implies something about the volatility of the species. It is very unlikely that the observed distributed sources for Cl and the refractory species are exclusively linked to the volatility of species on grains. The release of species in a distributed source is most probably a delayed release from (nano)grains, the process of which remains unknown at this time.

The mass calibration model developed during the project has indicated that additional corrections are necessary for an accurate direct mass calibration of mass spectrometers using a magnetic sector in space.

The creation of sum spectra has given us an additional tool to delve further in the data. Most of the species found could be linked to already known species or their isotopes. Unfortunately, not all discovered lowly abundant species have been conclusively identified yet. Further research on sum spectra and individual DFMS spectra will be needed.

Keywords

Comets, Cometary atmosphere, Rosetta mission, Gas analysis, Mass spectrometry