# MODELLING OF INFRARED SPECTRA OF COMETARY MOLECULES

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Comets are small icy bodies that are leftovers of the formation of the Solar system. As they are now located very far from the Sun, their composition have remained pristine, and they are considered fossils of our Solar system, containing crucial information about the conditions that prevailed nearly five billion years ago. The majority of comets observations are made from the ground when comets come closer to the Sun and start sublimating, revealing their inner composition through the formation of a coma.

Among the few space missions dedicated to cometary science, the spacecraft Rosetta launched in 2004 significantly improved our understanding of those small bodies, by studying the comet 67P/Churyumov-Gerasimenko for two years. One of the many instruments onboard the spacecraft, the mass spectrometer ROSINA led to the discovery of plenty of chemical species in the coma, that were never been observed in comets so far[1]. As space missions are rare, those detections must be generalized to ground-based cometary observations to improve our global understanding of comets.

In this framework, we present the modelling of two vibrational bands of chloromethane ($\nu_3$ and $\nu_6$) and one of cyanogen ($\nu_3$), two cometary molecules detected by ROSINA which are yet to be detected from ground-based observations. From high-resolution spectra obtained at the AIMES beamline of the SOLEIL synchrotron facility, positions and intensities of emission lines were derived and are freely available on the VAMDC portal[2]. These two molecules are the first ones to be studied in the context of the COSMIC project (Computation and Spectroscopy of Molecules in the Infrared for Comets), led by the EIPHI Graduate School[3]. From those databases, we intend to develop fluorescence models of those molecules in comets, and to search for their presence in high-resolution cometary spectra.

[1]Altwegg, K. (2017). Chemical highlights from the Rosetta mission. Proceedings of the International Astronomical Union, 13(S332), 153-162.

[2]https://vamdc.icb.cnrs.fr/

[3]https://gradschool.eiphi.ubfc.fr/?p=3710