Rotational Spectroscopy of Small Sulphur-Containing Radicals

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Molecular species with a dipole moment produce a unique rotational spectrum that is isomer, conformer, and isotopologue specific. The rotational spectra of molecules thus can be used as a fingerprint to help identify them in remote media such as the interstellar medium. Additionally, this spectral signature can be used to infer the physical properties of a system, such as its structure or the dynamics of any internal motion. In our group, we are continuously developing a range of spectroscopic techniques spanning from the microwave to the terahertz spectral regions for the characterisation of the rotation spectrum of molecules found, or likely to be found, in outer space. In this way, we hope to enable new interstellar detections of species playing a role in interstellar chemistry.

The experimental work is centred on two complementary spectrometers: a frequency multiplication-based absorption spectrometer employing lock-in detection of a frequency-modulated signal (75 – 900 GHz), and a chirped pulse Fourier transform spectrometer (75 – 110 GHz). The two spectrometers can be coupled with single or dual-pass samples cells, respectively, for the study of stable species, or a range of radical production techniques for the study of reactive species. The main radical production technique used in these experiments is hydrogen abstraction from a precursor molecule by atomic fluorine created by passing molecular fluorine through a microwave discharge. These experiments produce rich spectra, containing the rotational signatures of a range of interesting species. Experimental manipulation can help identify these species; for instance, the modulation of a magnetic field is used to discriminate between open-shell species and stable reaction products. An example of the previous application of these techniques is the characterisation of the spectrum of the CH_2OH radical from 140 to 330 GHz [1].

Currently we are working on producing spectral information on the CH_2SH radical, which lacks any published laboratory data. This work also involves characterising the spectra of other small sulphur-containing radicals such as HCS and H_3CS. To help with the identification of new species, we are implementing post-processing tools to help rapidly identify interesting spectral features. In the future, we will use a newly-built pulsed-jet experiment that will produce radical species cooled to below 10 K, for the sensitive detection of the transitions most relevant in cold environments such as molecular clouds in interstellar space.

[1] Chitarra, O. et al. *A&A* **644**, A123 (2020).