THZ SPECTROSCOPY FOR SPACE APPLICATIONS

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Advances in the generation of THz local oscillators (LOs) for ESA and NASA missions have enabled new techniques for THz spectroscopy. Furthermore, missions such as the Microwave Limb Sounder (MLS) and the Heterodyne Instrument for the Far Infrared (HIFI) have generated need for precise and accurate molecular spectroscopic parameters in the THz range. Multiplier chains have always been useful for locking fundamental millimeter and submillimeter oscillators such as Klystrons and Backward Wave Oscillators (BWOs). However the low power and poor spectral purity inhibited their usage as direct sources for spectroscopy. These two issues were mitigated in the efforts to provide stable, broadband LOs for the MLS and HIFI instruments. The resulting hardware is typically of similar power to a BWO, but has no requirements for external lock-loops or high voltage power supplies. The frequency generated is spectrally pure as long as the source frequency used to drive the chain is superb, and modulations can be applied directly at the source synthesizer. We have applied the Frequency Multiplier Submillimeter Spectroscopy (FMSS) technique to a wide range of spectroscopic problems over the last decade, including [1] Measurements of temperature dependent air-broadened linewidths [2] high-resolution broadband spectral characterization [3] narrow-band high resolution/high sensitivity integrations [4] pulsed/time resolved measurements (FT-THz), and [5] heterodyne spectrometry. These techniques will be discussed as will the active applications to research problems in space science such as: improving atmospheric composition measurements, characterizing interstellar interferant species, characterizing interstellar target species, studying non-LTE gases and developing analytical gas sensors.

HIGH RESOLUTION SPECTROSCOPY OF "INTERSTELLAR SPECIES" - FROM THE MICROWAVE TO THE FAR INFRARED.

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Laboratory studies of prospective and known interstellar species are essential to enable the assignment of the plethora of unknown lines in the mmwave region of the interstellar spectrum and so advance the understanding of the interstellar medium. It has been postulated that PAH variants containing one or more nitrogen substituents, the polycyclic aromatic nitrogen heterocycles (PANHs), may be responsible for variations in peak positions in IR interstellar emission features[1]. In order to provide data that could eventually unambiguously confirm the presence of such species in the ISM we have measured and assigned the pure rotational spectra of the 2 and 3 ring PANHs[2], Quinoxaline, quinazoline, phthalazine phenanthridine, acridine and 1,10phenanthroline employing Stark modulated millimetre wave absorption spectroscopy and FTMW spectroscopy of a supersonic rotationally cold molecular beam. Initial survey search scans were guided by rotational constants obtained through quantum chemical calculations performed at the B3LYP/6311G** level of theory with agreement well within 1% between the calculated equilibrium and experimentally derived ground state rotational constants. From the moments of inertia substantial negative inertial defects for all these species can be explained by the presence of several energetically low lying out of plane vibrational modes. Quadrupole coupling constants have been calculated from the FTMW data.

Many of the unknown interstellar lines in the mmwave region are postulated to be from vibrational satellites of molecules already discovered in the ISM and we have commenced a program investigating the low frequency modes of such species using long path cells on the far-IR high resolution spectroscopy beamline of the Australian synchrotron. An assignment and analysis of the highly coupled ν_8 (466.4550 cm^{-1}) and ν_{12} (409.0348 cm^{-1}) states of the short lived species ketenimine ($H_2C{=}C{=}NH$), where the observed lines of ν_{12} are purely by “perturbation allowed” transitions has been carried out to provide rotational, centrifugal and Coriolis interaction constants.

[1] D. M. HUDGINS, C. W. BAUSCHLICHER, L. J. ALLAMANDOLA, *Astrophys. J.,* **632**, 316 (2005)

[2] D MCNAUGHTON, P. D. GODFREY, R. D. BROWN, S. THORWIRTH, J.-Uwe Grabow, *Ap.J,* **678**, 309 (2008)