

A millimeter wave spectrometer on a chip for *in-situ* molecular spectroscopy Brian J. Drouin¹ A. Tang¹, E. Schlecht¹, A. W. Raymond^{1,3}, Mau-chung Frank Chang², Y. Kim², ¹brian.j.drouin@jpl.nasa.gov, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099 ²University of California, Los Angeles, Los Angeles, CA, 90095, ³Harvard University, School of Engineering and Applied Science, Cambridge, MA, 02138.

Introduction: Exploration of extra-terrestrial objects demands small, efficient investigative tools, ideally with highly specific and sensitive detections. Multiple science objectives outlined in the planetary science decadal survey [1] involve the detection of small molecular tracers and determination of their abundance and origin. For detections in the gas phase the rotational spectrum of a polar molecule typically provides a strong interaction with centimeter and shorter wavelength radiation, which has been exploited for remote sensing for half a century with data repositories growing to support these widespread efforts [2,3]. *In-situ* instruments are now being developed [4,5] but have lagged behind remote sensors due to the large equipment traditionally required for generation and detection of this radiation. These first generation instruments are man-portable, but not yet compact enough for space applications. Furthermore, the Fourier Transform microwave technique [6] has been utilized in research laboratories for three decades to determine fundamental physical properties of molecules and molecular complexes and extension of the technique to higher frequencies furthers study of the lightest molecules (*e.g.* hydrides) and complexes (particularly with Helium). Other research laboratories have built cavity resonators for sensitive detections in the millimeter [7] and submillimeter [8], however the injection losses reduce the potential to streamline the technique.

To realize the goal of a compact low-power system, we take advantage of new advances in both the transistor speed and size of commercial CMOS technology [9] that have enabled entire millimeter wave transmitters and receivers to be built on a single chip. This effort leverages these technological advances to enhance microwave techniques for *in-situ* gas detection. We have applied these advances in millimeter wave CMOS technology to standard microwave spectroscopic techniques [6,10] and realized the goal of developing a highly compact *in-situ* gas detection system. Extension of this technique into the millimeter had been slow due to difficulties with coupling radiation efficiently into high finesse cavities. Some exploratory work on wire-polarizer based coupling schemes have recently been described [11,12], but limitations of available hardware have precluded molecular detections. Extension of the traditional technique of incorporating back-fed coupled light directly behind a spherical mirror has reported sensitive detections at 59.1 GHz [13] and measurements up to 88 GHz have recently been

demonstrated [14], as well as a demonstration of the potential for cavity ringdown absorption spectroscopy at 94 GHz [7]. Our demonstrated method is similar to that proposed for mm-wave cavities by Braakman and Blake [11] except their wire grid coupler is replaced with a gold-plated coupler and the mm-wave light is created and detected at this coupler. The technique may be generally applicable across the THz spectrum and provides a template design for a multitude of planetary mission profiles. This instrumentation goal leaps forward in two important ways (1) there has not been an efficient means to a build cavity resonator for the millimeter and submillimeter wavelengths, and (2) the volume and mass of the electronics and optics (in comparison to traditional millimeter wave systems) decrease by more than an order of magnitude.

Results: In this first generation system, shown in Figure 1, the CMOS transmit and receive chips are demonstrated at the input/output interface of a planar coupler that injects the light into a semi-confocal Fabry-Perot cavity. The mirror position is adjusted to provide throughput in the range of one or more molecular resonances and light generated at the coupler interface is pulsed into the cavity.

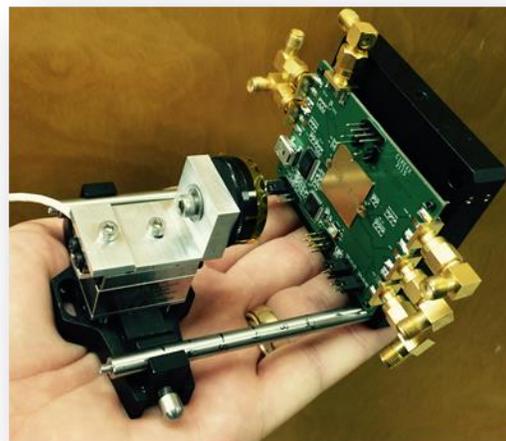


Figure 1. The CMOS devices that generate and receive the mm-wave radiation are each 1 mm². These are located on either side of the gold square (the coupler) on the circuit board. A 25 mm diameter, 25 mm focal length spherical mirror is positioned normal to the coupler plane on a precision translation stage that allows mode tuning across the 92-102 GHz bandwidth of the CMOS devices.

The mixer contains an embedded local oscillator tuned several MHz away from the resonance (and transmitted frequency) and the analog output of the mixer is fed to a digitizing oscilloscope for Fourier transform of the post-pulse echo response from molecules that are pumped into an excited state by the transmission pulse. An example of gas detection is shown in Figure 2. The CMOS circuitry draws only 250 mW of power during nominal operations, and total instrument power is dominated by the command/control hardware (USART and Atmega) that draw about 300 mW in the current configuration.

The example spectrum of N_2O allows an initial sensitivity derivation. Using an interaction volume of 0.2 cm^3 , the measured pressures and the signal to noise ratios (22 in center channel and integrating out over the width of the feature) of the measurements, we estimate the minimal detection for the system in its current configuration to be 5×10^{11} N_2O molecules, or 70 ppm in a 100 mTorr gas mixture for an integration time of 100 ms. Other molecules will have differing (typically lower) detection limits due to variation in dipole moment, which is very weak for N_2O (0.16 Debye).

Numerous volatile species are detectable in the bandwidth of the spectrometer, and efforts are underway to characterize the sensitivity to key molecular tracers that are relevant to planetary science including deuterated water and a variety of organic compounds. A system trade study is also underway that will examine trade-offs in the cavity dimensions. There is also a plan to miniaturize the data processing (CMOS analog to digital conversion as well as Fast Fourier Transform) to dramatically reduce the output bandwidth of the system without significantly increasing the power consumption.

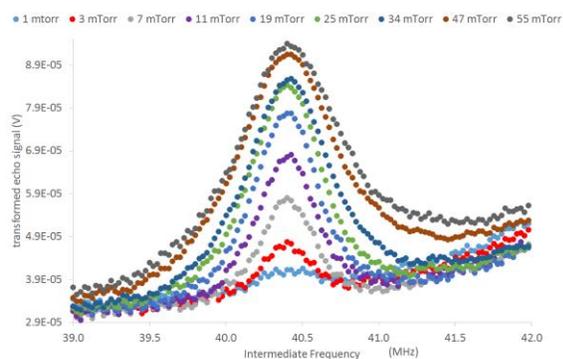


Figure 2. Data recorded with the system shown in Figure 1 embedded in a vacuum chamber with different gas flows of nitrous oxide (N_2O).

References:

- [1] Vision and Voyages for Planetary Science in the Decade 2013-2022, Committee on the Planetary Science Decadal Survey, Space Studies Board Division on Engineering and Physical Sciences, The National Academies Press, Washington, D.C.
- [2] H. M. Pickett, R. L. Poynter, E. A. Cohen, M. L. Delitsky, J. C. Pearson, and H. S. P. Mueller (1998) *J. Quant. Spectrosc. & Rad. Transfer* 60, 883.
- [3] H. S. P. Mueller, F. Schloeder, J. Stutzki, and G. Winnewisser (2005) *J. Mol. Struct.* 742, 215227.
- [4] Brian J. Drouin, Ken Cooper, Robert Dengler, Marcoanto Chavez, William Chun, Tim Crawford (2012) *Aerospace Conference, IEEE*, 3-10, 1 - 4.
- [5] Christopher F. Neese, Ivan R. Medvedev, Grant M. Plummer, Aaron J. Frank, Christopher D. Ball, and Frank C. De Lucia (2012), *IEEE Sens. J.*, 12.
- [6] T. J. Balle and W. H. Flygare (1981), *Rev. Sci. Instrum.* 52, 33.
- [7] N. Gopalsami, A.C. Raptis, J. Meier, Review of Scientific Instruments (2002), 73 (2) 259-262.
- [8] A.I. Meshkov and F.C. De Lucia, Review of Scientific Instruments (2005), 76 083103.
- [9] A. Tang, D. Murphy, F. Hsiao, G. Virbila, Y.-H. Wang, H. Wu, Y. Kim and M.-C. Frank Chang (2012) *IEEE Transactions Microwave Theory and Techniques IMS 2012 special issue*, 60 4129-4137.
- [10] R. N. Clarke and C. B. Rosenberg (1982) *J. Phys. E: Sci. Instrum.*, 15, 9-24.
- [11] R. Braakman, G.A. Blake (2011) *J. Appl. Phys.* 109, 063102.
- [12] B. A. DePrince, B. E. Rocher, A. M. Carroll, and S. L. Widicus Weaver (2013) *Review of Scientific Instruments* 84, 075107.
- [13] D. Halfen, L.M. Ziurys (2016) presentation WH03, International Symposium on Molecular Spectroscopy.
- [14] J. K. Anderson, D.T. Halfen, L.M. Ziurys (2015) *J. Mol. Spec.* 307, 1-5.

Additional Information: This material is based upon work supported by the National Aeronautics and Space Administration under Grant No. NN13D485T issued through the Planetary Science Division PICASSO program. AR is supported by NSTF grant NMX13AM67H. Portions of the research described in this paper were performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration, government sponsorship acknowledged.