

Quantum cascade laser spectrometer for trace-gas detection of exhaled Carbonyl Sulfide

Matt McCurdy, Gerard Wysocki, Chad Roller, Stephen So, Damien Weidmann, Robert F. Curl, and Frank K. Tittel

Rice Quantum Institute, Rice University

R. Bag, and M. C. Paraguya

Department of Pulmonary Medicine, Baylor College of Medicine

Department of Bioengineering

Rice University

Houston, TX 77251-1892

Phone: (713) 266 1422, Fax: (713) 348 5686

mccurdy@rice.edu

Detection and analysis of carbonyl sulfide (COS) is of importance in a number of applications which includes medical diagnostics. Elevated COS concentrations in exhaled breath has been reported recently in lung transplants recipients suffering from acute rejection [¹] as well as patients with liver disease [²]. The low parts-per-billion (ppb) concentration range of many volatile molecular species in human breath presents a novel approach and opportunity for clinical breath analysis, which requires rapid, *in situ*, detection of trace-gases. In contrast to current invasive diagnostic methods (e.g. bronchoscopic lung biopsies to assess acute lung rejection), rapid analysis of expired breath using mid infrared laser absorption spectroscopy (MIRLAS) is a desirable non-invasive alternative. In this work we report the development of a MIRLAS gas sensor utilizing a quasi room temperature pulsed QC laser for simultaneous detection of COS and carbon dioxide (CO₂) in expired breath. The sensor architecture is similar to the one reported in Ref. ³ and ¹. The thermoelectrically cooled QC laser operates in a pulsed mode at 4.85 μm and can be tuned between 2054.5 and 2060.5 cm⁻¹, which covers a number of strong absorption lines in the P branch of the COS fundamental vibrational-rotational spectrum. To minimize pulse-to-pulse fluctuations, reference and sample beam signals are monitored by means of a single photovoltaic HgCdTe detector and time resolved data acquisition electronics. The QC laser is driven by 25 ns current pulses with repetition rates of up to 500 kHz. Wavelength scanning is performed using fast modulation of the laser sub-threshold current. Feedback electronics is applied for stabilization of laser power fluctuations. This technique results in an improved signal-to-noise (S/N) ratio as well as stabilizing the laser linewidth. The absorption spectrum is digitized and recorded using a fast data acquisition card. The current noise equivalent sensitivity of the sensor is estimated to be ~10 ppb. In addition, trace gas sensor portability and fast data acquisition for better statistical noise cancellation is being developed using digital signal processing (DSP) technology.

The field of breath collection is in its infancy, and in the absence of standardization, various techniques have been used to collect samples that allow for analysis of different parts of the airway. Researchers using different techniques report conflicting results in the literature. In this study, we compare various breath collection techniques in the detection of COS.

¹ S.M. Studer, J. B. Orens, I. Rosas, J.A. Krishnan, K. A. Cope, S. Yang, J.V. Conte, P.B. Becker, and T. H. Risby, "Patterns and Significance of Exhaled-Breath Biomarkers in Lung Transplant Recipients with Acute Allograft Rejection", *J. of Heart and Lung Transplant*, 20(11), 1158 (2001)

5:00-6:30 pm, February 12, 2004, Shamrock Ballroom, University Hilton Hotel, Houston, 109
Texas