Rapid Spectroscopic Detection of Volatile Organic Compounds With Widely Electrically Tuneable Quantum-Cascade Lasers

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A fast, accurate, and in-situ detection of volatile organic compounds (VOCs) can be beneficial for quality control in many industrial fields, environmental monitoring, and medical diagnostics. Laser-absorption spectroscopy (LAS) has the potential to fulfil these requirements, even though VOCs exhibit broad and spectrally overlapped absorption spectra, but it requires light sources with broad spectral coverage. Extended-tuning quantum-cascade (QC-XT) lasers [1] are a promising candidate that can combine rapid, high-resolution spectral scanning with broad coverage.

In this work, we present the development and characterisation of a compact mid-IR spectrometer for the high-precision and simultaneous measurement of small VOCs. The analyser uses a QC-XT laser (Alpes Lasers) coupled to a multi-pass cell with 76 m of optical path. By means of the Vernier effect, the laser can be operated in six different spectral windows (each ~1.5 cm^{-1} wide) distributed between ~1163 cm^{-1} and ~1102 cm^{-1}. A complete spectrum is measured every 360 ms by rapid switching between and tuning within the six windows.

VOC measurements were performed in a flow-through configuration at low pressure (~50 mbar) to minimise the broadening of spectral lines. The spectra were recorded at high resolution (<10^{-4} cm^{-1}), which is not available in the literature for most VOCs. Thus, we generated our reference database and developed a concentration-retrieval algorithm.

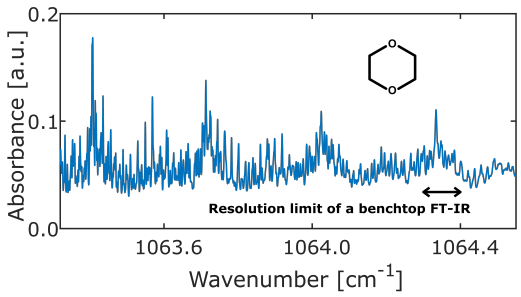

Figure 1. Absorption spectrum of 1,4-dioxane recorded in one of the spectral windows. Several VOCs, containing up to four carbon atoms (C4), reveal significant fine structure in their ro-vibrational spectrum. Such distinct narrow features were also observed for larger molecules (~C6) with rigid molecular structure or high-order symmetry.

Our instrument is well-suited for the detection of small oxygen-containing VOCs at amount fractions down to tens of ppb. We have achieved a typical precision of ~1 ppb for 25 s averaging time, demonstrated for methanol at an amount fraction of 10 ppm, and a large linearity range over 3 orders of magnitude. The broad measuring range, high spectral resolution, and the unique spectral fingerprints of the investigated VOCs assure excellent selectivity of the presented method. This enables multi-compound measurements and raises new possibilities for laser-spectroscopic analysis of VOCs.

The system is currently being further developed for breath analysis in the framework of Zurich Exhalomics [2].

[1] Y. Bidaux, A. Bismuto, C. Tardy, R. Terazzi, T. Gresch, S. Blaser, A. Muller, and J. Faist, *Appl. Phys. Lett.* **107**, 221108 (2015).
[2] https://www.exhalomics.ch/ (Accessed: 14.03.2022)