Trace gas detection: High resolution vibrational spectroscopy of atmospheric molecules

Dr Julia Lehman (SoC) and Prof Dwayne Heard (SoC)

Contact email: j.lehman@leeds.ac.uk

Alkyl peroxy radicals (RO_2) are important intermediates in a variety of atmospheric processes, such as the oxidation of NO to form NO_2 (whose subsequent photolysis leads to the formation of tropospheric ozone). However, simple alkyl peroxy radicals, such as methyl peroxy, have yet to be observed in field studies. While the FAGE technique developed here at the University of Leeds offers excellent sensitivity (Onel *et al., Atmos. Meas. Tech.,* 2017, 10, 3985), it relies on an indirect multistep process to characterize the abundance of alkyl peroxy radicals, determined through chemical reaction and subsequent laser-induced fluorescence, and can lack RO_2 specificity.

Objectives:

In this project, you will work with a direct detection technique and benchmark the new apparatus against the FAGE technique. You will measure high resolution vibrational absorption spectra at room temperature using a cutting-edge laser-based detection method: cavity-enhanced mid-infrared frequency comb vibrational absorption spectroscopy. As demonstrated by the Ye group at JILA, University of Colorado, Boulder, USA (Bjork *et al., Science*, 2016, 354, 444), cavity-enhanced frequency comb spectroscopy can be used to simultaneously obtain a broadband and high-resolution vibrational absorption spectrum. You will apply this technique to measure the vibrational absorption spectra of several alkyl peroxy radicals, working towards increasing sensitivity and selectivity. You will interpret the laboratory measurements with the aid of theoretical methods, including quantum chemical calculations and spectroscopic modelling.

Potential for high impact outcome

It is anticipated that this project will generate several papers, with potential for publication in high impact journals.

Training

The student will work under the supervision of Dr Julia Lehman and Prof Dwayne Heard within the Atmospheric and Planetary Chemistry group in the School of Chemistry at the University of Leeds. You will be supported by a range of supervisions from monthly meetings and group presentations, through to daily informal chats with supervisors. You will work in well-equipped laboratories and be part of an active, thriving and well-funded atmospheric chemistry community. The Leeds group receives funding from the National Centre for Atmospheric Science (NCAS) and is part of the Atmospheric Measurement Facility, and has an internationally leading reputation in atmospheric chemistry for field measurements of atmospheric composition, laboratory studies of chemical kinetics and photochemistry, and the development of numerical models and chemical mechanisms, including the Master Chemical Mechanism (MCM, Saunders *et al.*, 2003; Jenkin *et al.*, 2003). Activities in these three areas are intimately linked and interdependent, providing significant advantages. You will be supported to attend both national and international conferences, and will receive a wide range of training, for example in communication skills, project management, and with

other technical aspects (for example LabView and computing). This PhD will provide a broad spectrum in training, particularly covering vibrational absorption spectroscopy, kinetic methods, high-resolution laser-based spectroscopic techniques, optics, vacuum systems, and quantum chemical calculations. You will also receive training in writing and implementing computer controlled data acquisition and analysis programs. You will also have access to training provided by the National Centre for Atmospheric Science such as the Arran Instrumental Summer School and other courses. The successful PhD student will have access to a broad spectrum of training workshops that include managing your degree and preparing for your viva (http://www.emeskillstraining.leeds.ac.uk/).

Student profile

The student should have an interest in atmospheric chemistry, air quality and global environmental problems, with a strong background in experimental physical chemistry or similar (e.g. physics, engineering, environmental science). Standard NERC eligibility rules apply.

References

Onel *et al.*, *Atmos. Meas. Tech.*, 2017, 10, 3985

Bjork *et al.*, *Science*, 2016, 354, 444