Selected Research Topic number: **SRT-v01** Version: 1.0



Title: Traceable spectral data for atmospheric monitoring

Abstract

Spectro-analytical techniques are indispensable for atmospheric remote sensing. Their key datasets are species-specific traceable spectral data, which serve as an inherent transfer standard and are required to ensure traceability. The identified requirement is to determine and disseminate traceable gas phase spectra of essential atmospheric species, including the determination of precision isotopologue spectra, high line density spectra, absorption cross sections of heavy molecules, reference spectra in the UV/VIS, the improved generation of reference gases for isotopologues and reactive species, and the metrological evaluation and improvement of field FTIR retrievals.

Conformity with the Work Programme

This Call for JRPs conforms to the EMRP Outline 2008, section on "Grand Challenges" related to Energy and Environment on pages 9, 24, 25 and 40.

Keywords

Spectroscopic data; laser spectroscopy; FT-IR; atmospheric measurements and remote sensing; ground-based, satellite and airborne sensor networks, climate change, air quality, European infrastructure

Background to the Metrological Challenges

Traceability of the spectroscopic data under a wide range of pressure and temperatures, which underlies the majority of technologies used to monitor the atmospheric climate, is absolutely essential in order to ensure comparability over the long time scales and long range spatial coverage necessary to detect climatic changes. Further, global atmospheric monitoring networks always consist of a broad range of diverse instrument types that are distributed over huge areas. The large size of sensor networks is necessary to cover global climatic effects and discern those from local events.

Continuing technological advances made in the remote sensing methods used are allowing increasing types, and ranges of data to be collected, analysed and disseminated for environmental modelling. This is further increasing the demand for metrological grade spectral data to new species and matrix range of temperatures and pressures under which the data is measured.

Despite the significant efforts in the past to determine the required spectral data and to setup and maintain spectral line-by-line data bases, LBLDB, (like HITRAN or GEISA) for their dissemination, the situation remains unsatisfactory in the sense that an almost negligible part of the large body of the spectral data available in the literature or in LBLDB, has been determined in a traceable fashion and generally without a rigorous error analysis, and rarely seen with an uncertainty budget according to metrological principles such as the GUM.

Scientific and Technological Objectives

Proposers should address the objectives stated below, which are based on the PRT submissions. Proposers may identify amendments to the objectives or choose to address a subset of them in order to maximise the overall impact, or address budgetary or scientific / technical constraints, but the reasons for this should be clearly stated in the JRP-Protocol.

The JRP shall focus on traceable precision measurements of molecular spectral data for environmental monitoring.

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The specific objectives are

- Measurement of spectral reference data in the NIR/MIR region for: a new set of important atmospheric species (e.g. NH₃, NO₂, HNO₃, VOC, CH₂O, SF₆, C₂- and C₃- Hydrocarbons, Cl-, F-, Br-containing hydrocarbons and halides); important isotopologues of GHG (eg CO₂, CH₄, N₂O, ^{14/15}N- ratios); heavier molecules, with high line density and partially resolved or unresolved rotational; and chemically reactive or instable molecules (eg NH₃, NO₂, HNO₃).
- 2. UV/VIS spectral reference data measurements (e.g. for NO₂, SO₂, O₃, Cl-, F-, Br-oxides)
- 3. Improvement of the metrological description of molecular spectra under varying pressure, temperature, matrix conditions by: developing and improving means to traceably determine over the full range of the environmental range of boundary conditions (i.e. 180 to 350 K, 0 to 0.11 MPa) for a range of spectral features (e.g. temperature and pressure dependence of line position and strength); and investigating suitable line shape models to better describe line broadening, and in particular line mixing and collisional narrowing.
- 4. Development of essential supporting infrastructure for traceable spectral data measurement, for example: preparative and analytical capabilities for isotopically defined stable reference gases; and optical transfer standards for the traceable dynamic analysis of reactive or instable gases.
- 5. Development of metrological procedures for atmospheric monitoring retrievals of groundbased FTIR networks and active transfer of traceable spectral data to such applications.

These objectives will require large-scale approaches that are beyond the capabilities of single National Metrology Institutes and Designated Institutes. To enhance the impact of the R&D work, the involvement of the user community such as industry, and standardisation and regulatory bodies, as appropriate, is strongly recommended.

Proposers should establish the current state of the art, and explain how their proposed project goes beyond this. In particular, proposers should outline the achievements of the EMRP project ENV06 "EUMETRISPEC" and how their proposal will build on those. Acknowledging the huge number of species, which are relevant for environmental monitoring, the proposers shall describe how the European metrology community may prioritise the species to be addressed in the long term, and what a sustainable infrastructure for spectral reference data might look like.

EURAMET expects the average size of JRPs in this call to be between 3.0 to $3.5 \text{ M} \in$, and has defined an upper limit of 5 M \in for any project. The available budget for integral Research Excellence Grants is 30 months of effort.

Potential Impact

Proposals must demonstrate adequate and appropriate participation/links to the "end user" community. This may be through the inclusion of unfunded JRP partners or collaborators, or by including links to industrial/policy advisory committees, standards committees or other bodies. Evidence of support from the "end user" community (eg letters of support) is encouraged.

You should detail how your JRP results are going to:

- be taken up by the environmental monitoring community.
- If appropriate, feed into the development of urgent documentary standards through appropriate standards bodies

You should detail other impacts of your proposed JRP as detailed in the document "Guide 4: Writing a Joint Research Project"

You should also detail how your approach to realising the objectives will further the aim of the EMRP to develop a coherent approach at the European level in the field of metrology and includes the best available contributions from across the metrology community. Specifically the opportunities for:

- improvement of the efficiency of use of available resources to better meet metrological needs and to assure the traceability of national standards
- the metrology capacity of Member States and countries associated with the Seventh Framework Programme whose metrology programmes are at an early stage of development to be increased
- outside researchers & research organisations other than NMIs and DIs to be involved in the work

Time-scale

The project should be of up to 3 years duration.