Molecular spectroscopy: towards accurate reference parameters for atmospheric applications

Katarzyna Bielska

Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University in Toruń

Remote sensing based on spectroscopic techniques delivers a variety of information about the Earth atmosphere, such as pressure and temperature profiles [1], clouds parameters [2], and its chemical composition needed for tracking and understanding climate changes [3], identifying sources and kinds of pollutants [4], and providing data on the air quality [5].

Many of the above applications require high measurement accuracy, which cannot be achieved without high-quality reference data regarding positions, intensities, and the shape of spectral lines [6,7]. Over the years, a vast amount of spectral data has been collected and stored in spectral databases, such as HITRAN [8]. However, in many cases, the data quality is relatively low: sub-percent accuracy requirements of the remote sensing meet data with line intensities characterized by few-percent uncertainties and incomplete sets of lineshape parameters.

Additional difficulty regarding atmospheric applications results from very long absorption path lengths. It causes a demand for reference data regarding low-intensity absorption bands, which are challenging in laboratory measurements. Such measurements often require absorption path enhancement with the use of optical cavities. Also, the most accurate measurement techniques, such as cavity ring-down spectroscopy [9], cannot provide a sufficiently large datasets. The last issue can be solved through the effective collaboration between experimental and theoretical groups, which may lead to predicting spectral parameters for unmeasured transitions if high-quality experimental data is used to support theoretical calculations [10]. I will present some of the most accurate measurement techniques applied to molecules of atmospheric importance, such as oxygen, carbon monoxide, and carbon dioxide, both in Doppler-limited and Doppler-free regime.

1. C. R. Nowlan et al., J. Quant. Spectrosc. Radiat. T. 108 (3) (2007) 371
2. A. Kuze, K. V. Chance, J. Geophys. Res. 99 (D7) (1994) 14481
3. A. Voulgarakis et al., Atmos. Chemis. Phys. 13 (2013) 2563
4. J. A. Logan et al., J. Geophys. Res. 86 (1981) 7210
5. C. Zhang et al., Light-Sci. Appl. 8 (2019) 100
6. D. R. Thompson et al., J. Quant. Spectrosc. Radiat. T. 113 (2012) 2265
7. R. A. Washenfelder et al., J. Geophys. Res. Atmos. 112 (2006) 1
8. I. E. Gordon et al., J. Quant. Spectrosc. Radiat. T. 203 (2017) 3
9. A. O'Keefe and D. A. G. Deacon, Rev. Sci. Instrum. 59 (1988) 2544
10. O. L. Polyansky et al., Phys. Rev. Lett. 114 (2015) 243001