



Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: 2540

Type: Oral (Non-Student) / Orale (non-étudiant(e))

Do the temperature dependencies of spectral line parameters change when we approach cryogenic temperatures?

Monday, 3 June 2019 14:15 (15 minutes)

We have recently studied a set of 40 spectra of carbon monoxide in pure state and mixed with air, recorded at temperatures between 79 to 296 K. Our aim was to investigate if the temperature dependencies of line parameters, such as half widths and pressure induced shifts, stay the same at very low temperatures, close to 79 K. The spectra were all recorded over two decades using the 1-m Fourier Transform spectrometer located at Kitt Peak, AZ, USA and two temperature controlled gas cells. The spectra were calibrated using the line positions for residual carbon dioxide and water vapour and referencing them to the HITRAN database.

The constrained analysis technique was used together with the software Labfit [2]. Three line shape models were employed: Voigt, speed-dependent Voigt and Rautian. In the absence of experimental narrowing parameters, we have calculated them using computed diffusion constants [3].

The theoretical half-width coefficients for CO-N₂ have been determined at several temperatures employing a potential energy surface of Tipping-Herman type, vibrationally independent potentials and by taking into account the electrostatic interactions. We will discuss what laws were found to best represent the temperature dependencies over a wide range of temperatures, approaching cryogenic temperatures.

We thank D. Chris Benner for the Labfit software. The work of V.M. Devi was funded by NASA grants and contracts, and the research by M. A. H. Smith was performed as part of her employment at NASA Langley Research Center. No official endorsements are intended or implied. N. Islam and A. Predoi-Cross have been funded by NSERC. S. Ivanov and O. Byzykin received financial support from the Ministry of Science and Higher Education within the State assignment FSRC «Crystallography and Photonics» RAS and Russian Science Foundation (Project No.18-55-16006).

References:

1. I.E. Gordon, L.S. Rothman, C. Hill, R.V. Kochanov, Y. Tan, P.F. Bernath, et al. *J. Quant. Spectrosc. Radiat. Transfer* 203, 3–69 (2017).
2. D.C. Benner, C.P. Rinsland, V.M. Devi, M.A.H. Smith, D. Atkins, *J. Quant. Spectrosc. Radiat. Transfer* 53(6), 705-721 (1995).
3. J.O. Hirschfelder, C.F. Curtiss, R.B. Bird, *Molecular theory of gases and liquids*. New York: Wiley and Sons, 1952.

Primary authors: PREDOI-CROSS, Adriana (University of Lethbridge); Mr ISLAM, Nazrul (University of Lethbridge); Dr SMITH, Mary Ann (Science Directorate, NASA Langley Research Center); Dr DEVI, Malathy (Department of Physics, The College of William and Mary); Dr IVANOV, Sergey (Institute on Laser and Information Technologies, Russian Academy of Sciences); Dr BUZYKIN, Oleg (Central Aerohydrodynamic Institute (TsAGI)); Prof. THIBAUT, Franck (Université de Rennes)

Presenter: PREDOI-CROSS, Adriana (University of Lethbridge)

Session Classification: M2-1 Interaction Between Matter and Light (DAMOPC) | Interaction de la matière et de la lumière (DPAMPC)

Track Classification: Division of Atomic, Molecular and Optical Physics, Canada / Division de la physique atomique, moléculaire et photonique, Canada (DAMOFC-DPAMPC)