EPSC Abstracts
Vol. 6, EPSC-DPS2011-115, 2011
EPSC-DPS Joint Meeting 2011

Theoretical modelling of the methane absorption spectrum for planetary applications

V. Boudon (1), A. Nikitin (2), T. Gabard (1), Ch. Wenger (1), M. Rey (3) and Vl. G. Tyuterev (3)
(1) Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9. Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France (Vincent.Boudon@u-bourgogne.fr), (2) Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics, Russian Academy of Sciences, 634055 Tomsk, Russia, (3) Laboratoire GSMA, UMR 6089 CNRS–Université de Reims Champagne-Ardenne, Moulin de la Housse, BP 1039, Cases 1617, F-51687 Reims Cedex 2, France

Abstract

Methane is a key species in many planetary atmospheres, including Titan, the giant planets and exoplanets. In this paper, we present the state-of-the-art of line-by-line (line positions, line intensities and line broadening) modeling of the CH_4 infrared absorption spectrum. We also discuss the perspectives and future directions of this topic.

1. Introduction

The methane molecule (CH_4) is the simplest of saturated hydrocarbons. This chemical species is relatively abundant in the Universe. On Earth, it is the main constituent of natural gas and is the second greenhouse gas (after carbon dioxide) for which emissions should be urgently reduced, as recommended by the Kyoto protocol. Methane is also present in quite important proportion in the atmosphere of a number of extraterrestrial objects: the giant planets of the Solar System (Jupiter, Saturn, Uranus and Neptune), but also Mars, Titan (Saturn's main satellite), Triton (Neptune's main satellite), Pluto and Kuiper Belt objects and, farther away, brown dwarfs, some "cold" stars and giant exoplanets ("hot jupiters").

2. Modelling the methane spectrum

For all these applications, it appears that the methane spectrum is still insufficiently known, especially in the near infrared and visible regions. Since many years, the Dijon group has developed a specific model and tools for the analysis and modeling of the spectrum of this kind of highly symmetrical molecules. It is now part of the French ANR project "CH_4@Titan" that gathers both experimentalists recording methane laboratory spectra, theoreticians doing spectrum modeling and planetologists that are specialists of Titan's atmosphere.

3. Line positions and intensities

We will present here the specificities of the methane spectrum, as well as the characteristics of the "Dijon model". Then, we will detail the present state of the modeling of CH_4's spectrum along with some applications to planotology.

Vibrational levels of methane are grouped into packets called polyads. We will especially insist on the state-of-the art of the line-by-line global analysis [1] for the $^{12}CH_4$ main isotopologue. The latest results, to be published soon, and concerning the so-called Tetradecad region near 1.6 µm (see Figure 1) will be shown. A recent reinvestigation of the ground state rotational line intensities [2] will also be discussed. The case of the $^{13}CH_4$ and $^{12}CH_3D$ isotopologues will be mentioned too.

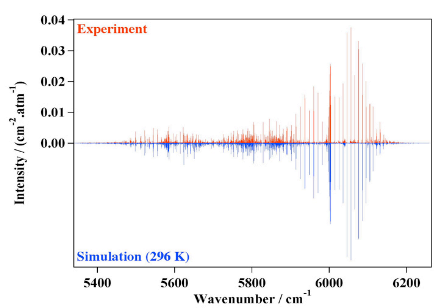

Figure 1: Global comparison between experiment and simulation for the Tetradecad region at 296 K.

4. Line broadening

Line shape modelling is also essential for applications to planetary atmospheres, which are heterogeneous environments with several molecules mixed.

We present an original semi-classical method [3], without any adjustable parameter. It allows collisional broadening coefficient calculation for methane with different gas perturbers (including nitrogen N_2, see Figure 2).

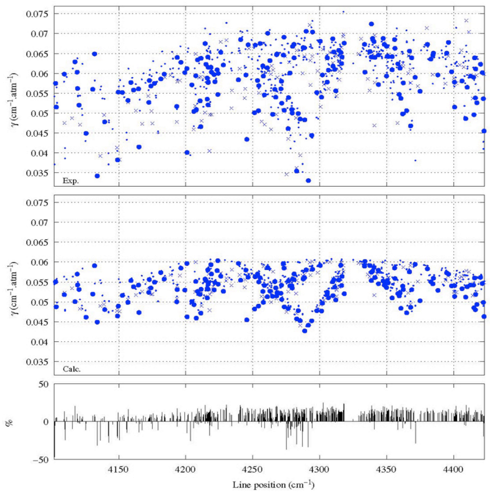

Figure 2: Comparison between experiment and theory for nitrogen broadening coefficients in the Octad region.

5. Future directions

Higher polyads being extremely complex and almost intractable for line-by-line assignments, new theoretical approaches should be developed. We propose a new innovative method allowing to deduce effective operators (Hamiltonian and dipole moment) from *ab initio* surfaces.

The so-called "spectroscopic" effective Hamiltonians to be used for data reductions and predictions at high energy range could be systematically built by generalized Contact Transformations [5] from accurate potential function [6].

6. Summary and Conclusions

There is still a considerable work to perform on the modeling of the methane spectrum, in order to reach all requirements for planetary and stellar applications. In particular, the study of hot objects, like giant exoplanets and brown dwarfs, implies the study of highly excited states. All this requires both new theoretical and experimental efforts.

All the results and line lists resulting from our work will be made available to the scientific community though the VAMDC (Virtual Atomic and Molecular Data Center) interface, presently under construction. A methane line list server with a preliminary user interface is already set-up in Dijon [4] in this framework.

Acknowledgements

This work is part of the French ANR Project ''CH4@ Titan'' (Ref: BLAN08-2_321467, see http://icb.u-bourgogne.fr/titan/) and of the VAMDC European network (http://www.vamdc.org).

References

[1] Albert, S., Bauerecker, S., Boudon, V., Brown, L. R., Champion, J.-P., Loëte, M., Nikitin, A., and Quack, M.: Global analysis of the high resolution infrared spectrum of methane $^{12}CH_4$ in the region from 0 to 4800 cm^{-1}, Chemical Physics, Vol. 356, pp.131-146, 2009.

[2] Boudon, V., Pirali, O., Roy, P., Brubach, J.-B., Manceron, L., Vander Auwera, J.: The high-resolution far-infrared spectrum of methane at the SOLEIL synchrotron, Journal of Quantitative Spectroscopy and Radiative Transfer, Vol. 111, pp. 1117-1129, 2010.

[3] Gabard, T., and Boudon, V.: Line broadening coefficient calculations for methane perturbed by nitrogen, Journal of Quantitative Spectroscopy and Radiative Transfer, Vol. 111, pp. 1328-1343, 2010.

[4] http://vamdc.icb.cnrs.fr/PHP/methane.php

[5] Tyuterev, Vl. G., Tashkun, S. A., Rey, M., Kochanov, R. V., Nikitin, A. V., HRMS Dijon 2011.

[6] Nikitin, A. V., Rey, M., Tyuterev, Vl. G., Chemical Physics Letters, Vol. 501, pp 179-186, 2011.