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Spectroscopy and planetary atmospheres/Spectroscopie et atmosphères planétaires

Infrared spectroscopy of planetary atmospheres

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Abstract

Spectroscopy is at the root of modern planetology, in that it gives access remotely to the possibility to analyze the physical properties of planets. Today, the spectacular advance in techniques and models available to planetology reach an accuracy giving access to new domains in planetary physics, as meteorology, physico-chemical processes, etc. This article is centred on the infrared spectroscopy techniques. It will describe some of the physical observables accessible to modern instrumentation, in space or from the ground. The theoretical as well as instrumental limitations will be given, and the expected progress in short or medium term will be described. ***To cite this article: P. Drossart, C. R. Physique 6 (2005).***

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Résumé

Spectroscopie infrarouge des atmosphères planètes. La spectroscopie a véritablement fondé la planétologie moderne en permettant d'analyser les propriétés physiques des planètes à distance. Aujourd'hui, les progrès spectaculaires des techniques et des modèles disponibles atteignent aujourd'hui une précision qui rend accessible des pans entiers de la physique planétaire (météorologie, processus physico-chimiques, etc.) Cet article, centré sur les techniques de spectroscopie infrarouge, décrira quelques unes des observables physiques accessibles par les instruments actuels, dans l'espace ou au sol, les limitations tant théoriques qu'instrumentales, et les avancées à attendre à court et moyen terme. ***Pour citer cet article : P. Drossart, C. R. Physique 6 (2005).***

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Mots-clés : Spectroscopie infrarouge ; Planètes ; Abondances ; Rapports isotopiques

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1. Introduction

Spectroscopy is one of the most useful tools for the astrophysicist observing remotely physical properties of the bodies studied. In that sense, it has given planetology many opportunities, well before the space age. The detection of methane and ammonia on Jupiter and Saturn in 1932 [1] can therefore be considered as the foundation of physical planetology, aimed at understanding planets beyond a phenomenological description. This paper intends to give an overview of some recent results obtained from space or ground-based observatories, about different planets. An exhaustive description of the questions raised by spectroscopic measurements is out of scope of this paper, but several questions will be introduced, in order to indicate the present limitations, both technological and spectroscopic. This frontier in planetary research will give the reader an idea of the current and future efforts which will be necessary to go forward.

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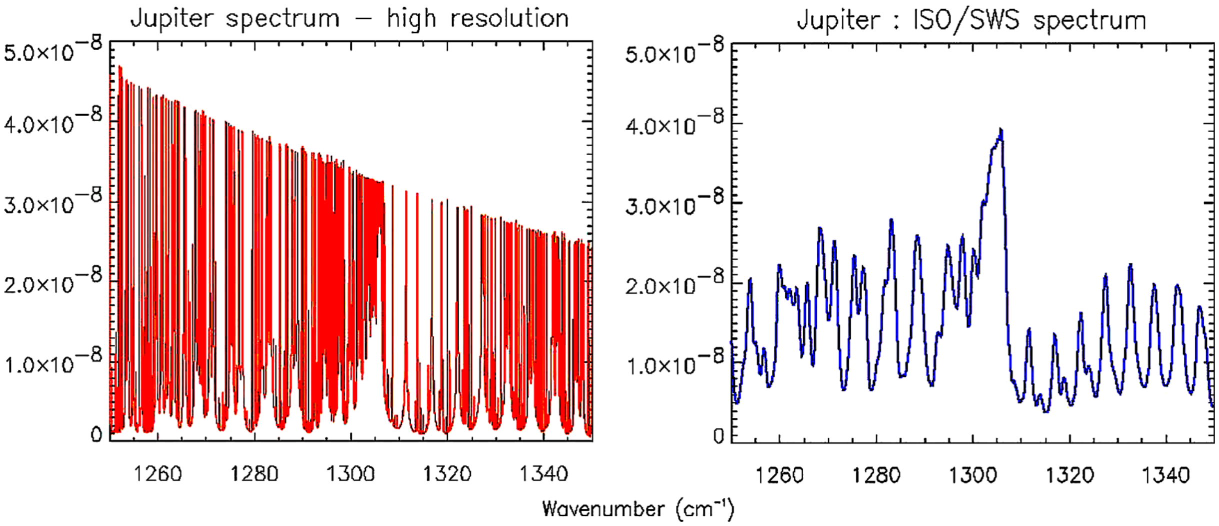

Fig. 1. Synthetic spectrum at high resolution of thermal emission of methane on Jupiter. Left: calculated spectrum at ∼ 0.001 cm^{-1}. Right: convolved spectrum at a spectral resolution equivalent to ISO/SWS instrument (1 cm^{-1}).

2. Scientific objectives

There are many parameters directly or indirectly accessible to spectral analysis in planetary spectra: composition, pressure, temperature, thermal equilibrium, cloud structure, wave activity, etc. Almost every physical phenomenon of influence on the radiative transfer of a planet can be used, then possibly measured, from a variation of a dedicated spectral features. The remaining difficulties are to extract quantitative information, combining spectral, instrumental and astrophysical expertises. Two main limitations to spectral observations can increase the difficulties:

- spectral heterogeneity (Fig. 1): high spectral resolution planetary spectra have by essence a high intrinsic complexity. Even if low spectral resolution observations, due to instrumental limitations, seem to reduce this complexity, it is, in fact, only masking the real details, with a risk of ambiguity in the interpretation;
- spatial heterogeneity (Fig. 2): planetary spectra averaged over the full disk are integrating very inhomogeneous regions. Non-linearity in the observed physical phenomena can make an accurate inversion of a real physical parameter impossible, when it is processed from an averaged observation.

The combination of a highly resolving instrument, both spectrally and angularly, remains exceptional, and compromises are often needed. Such a combination can, nevertheless, be expected to produce new developments in planetary spectroscopy, as some recent instrumentation developments anticipate.

Although the spectral domain of planetary interest covers all the electromagnetic range, from radio waves to X-rays, this paper will be limited to the infrared spectroscopy domain. The different spectral ranges cover spectral transitions of different origins: electronic bands in ultraviolet, vibrational in the infrared and rotational in millimetre range. The infrared domain has the advantage of a great accessibility in ground-based observations, compared to UV, and is not limited to polar molecules with a rotational spectrum in the millimetre range. The planetary phenomena and the interpretation models are anyway similar between the different domains, and their complementarities give access to planetary atmospheres at very different depths, from different wavelengths range.

2.1. Radiative transfer methods

Radiative transfer techniques for planetary atmospheric studies were derived from Earth observation spectral models, as developed in the 1960s, after the first space observations [2]. Nevertheless, several simplifications have in general to be introduced in the models, depending on the needed accuracy, or also, unfortunately, the level of knowledge in the existing spectral data available. The radiative transfer equation in its most elementary form can be reduced to an integral over the radiative intensity of the external solar flux, in the solar reflected component domain, below approximately 4 microns, or over the intrinsic thermal flux beyond. The usual basic approximation takes a classical approach for radiative flux (thus neglecting interference effects), with quantum effects included only in the molecular absorption/emission processes. As will be seen from some examples,

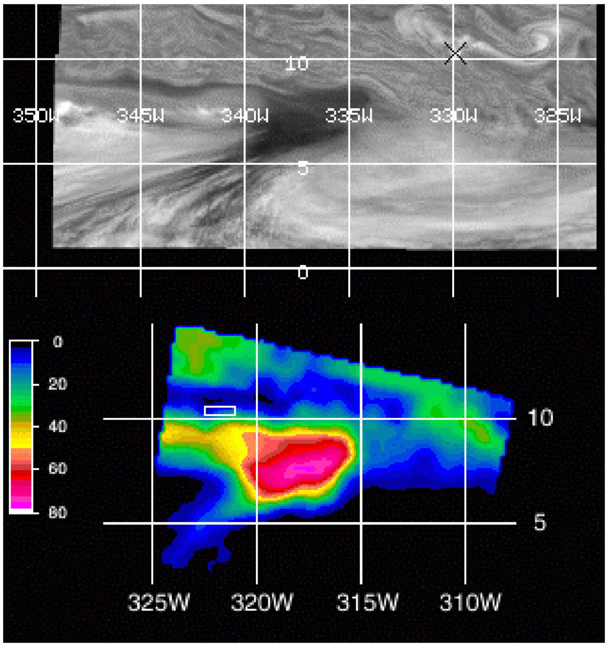

Fig. 2. Jupiter images in the visible (top) and in infrared at 5 micron (bottom) from Galileo spacecraft [11]: a large heterogeneity, both in the thermal and solar reflected component makes the spectral interpretation possible only with high spatial resolution.

this approximation is for planetary modelling largely satisfied, with possible discrepancies much lower than instrumental or modelling errors, with only rare exceptions.

2.1.1. Continuum

Outside the spectral absorption bands, the planetary spectrum is modulated by cloud effects (solar reflection over cloud layers, or thermal emission from these layers), or, in the thermal range, by the influence of far wings of molecular bands or pressure induced emissions [3]. On the giant planet spectra shown in Fig. 3, the pressure induced absorption due to the rotational spectrum of H_2, produced by collisions, is responsible to the general shape of the spectrum between 8 and 13 micron, when molecular absorption by CH_4 and NH_3 in particular form the emission or absorption bands seen in the spectrum. The interpretation of Voyager/IRIS observations of Jupiter [4] made great advances in the modelling of these continuum.

2.1.2. Spectral data

The molecular spectroscopy developments were spectacular in the interpretation of the planetary spectra due to the ever finer knowledge of the spectral parameters.

The physical parameters determination in the spectral bands is essential to the radiative transfer models, especially the line-by-line models which are currently the most accurate [2].

The description of each spectral band usually involves several hundreds to several thousands individual spectral lines, in order to give a reasonably accurate model of a planetary spectrum. The information needed for calculation on each individual line is the following:

- Line position;
- Line intensity;
- Broadening coefficient from major planetary constituents.

Other parameters are:

- Line shift, due to collisions are often neglected, because they appear at pressure levels where broadening largely dominates the spectral shift;
- Non-Lorentzian cut-off: this effect, related to the finite duration of a collision (as a Lorentzian shape is deduced from instantaneous collisions of molecules). A non-Lorentzian spectral profile introduce an overestimate of the continuum due

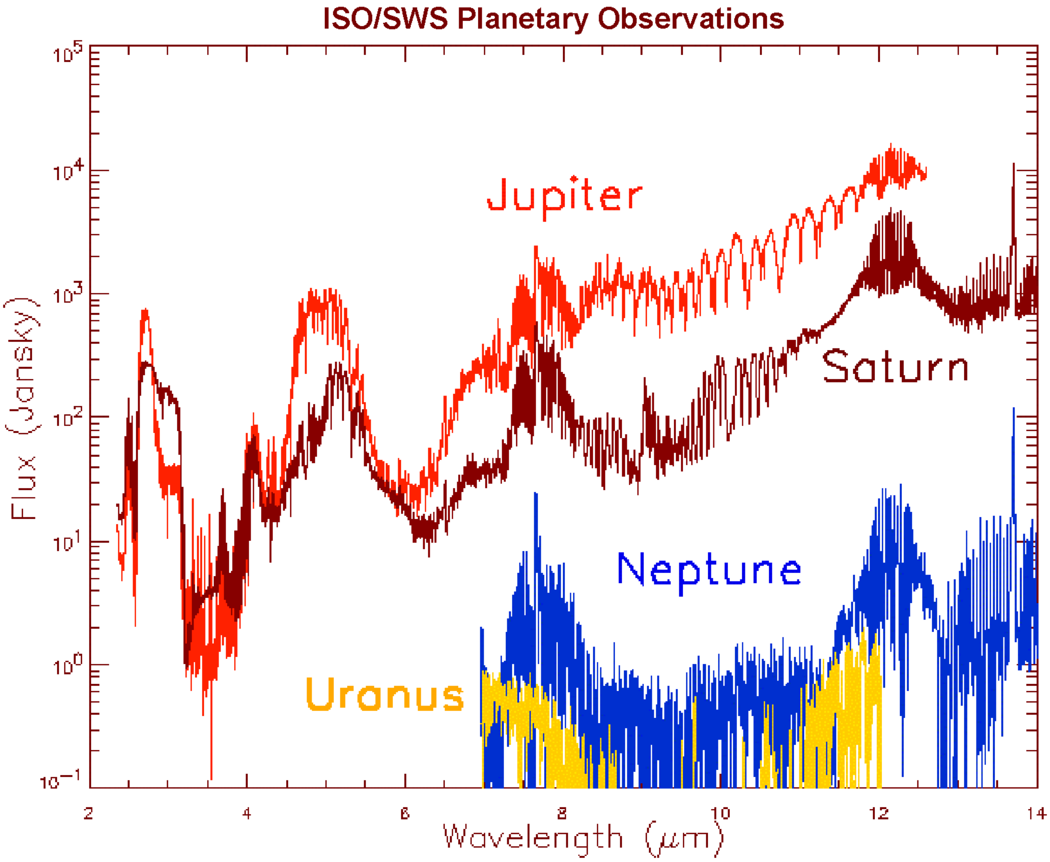

Fig. 3. Spectra of giant planets from ISO/SWS observations [12,13].

to far wings; approximate methods introduced to take this effect into account are to use a cut-off, beyond a certain distance from the line centre;

- Non-Lorentzian shape: this is a difficult field, which moreover introduces an overcomplexity in the radiative transfer calculation, and is still poorly explored in planetary atmospheric research [5]; an estimate of the uncertainties related to the use of an approximate model shows that only very high spectral resolution observations are expected to be sensitive to this effect in the infrared. Planetary models are in this sense far less sophisticated than terrestrial atmospheric models, where such effect are taken into account in meteorological or climatological models;
- Interference effects, line mixing: these effects are largely unexplored in planetary physics yet, and could concern only several specific features, like the Q branch of strong CH_4 bands in giant planets [6], or of CO_2 on Venus.

2.1.3. Non-LTE calculations

When calculations extend out of thermodynamic equilibrium (non-LTE) regime [7], other spectroscopic parameters are needed: the equation of radiative transfer includes in such a case equilibrium between radiative and collisional transitions, and collisional rates between the present chemical species have to be known. Relatively well known is the case for methane in giant planets [8], with principal collisions between CH_4 and H_2, and Titan (CH_4/N_2). Fig. 4 shows a synthetic calculation comparing Infrared Space Observatory / Short Wavelength Spectrometer (ISO/SWS) observations of the fluorescent emission of CH_4 in the Jupiter's atmosphere. These calculations rely on accurate knowledge of collisional and radiative coefficients.

2.1.4. Approximate models

Other approximations are often needed, either to limit the computation time of the radiative transfer, or simply because of unknown parameters:

- Average value for the broadening coefficient of all the lines within a band;
- Non-Lorentzian line shape approximated by a cut-off above a certain distance to the line centre [8].

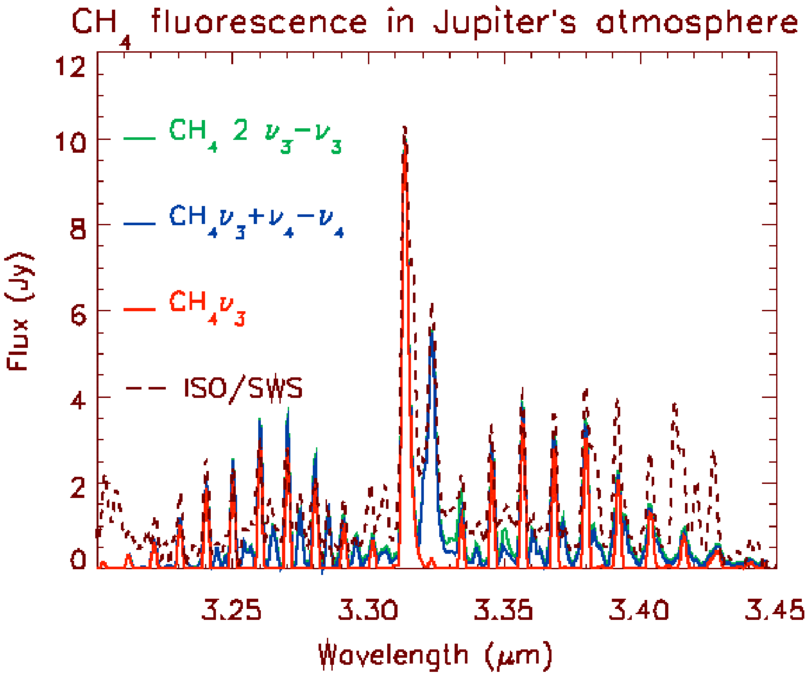

Fig. 4. Fluorescence of methane observed in Jupiter's atmosphere with ISO/SWS.

These approximations can in principle be justified due to the expected accuracy of the modelling, rarely better than 10%, due to imperfect knowledge of the planetary models themselves, or to the signal to noise limitations. With ever increasing accuracy of modern observations, it is certain that future modelling will need to go beyond such approximations, as it was the case for Earth models in the past.

The most accurate direct models, line-by-line calculations, are integrating directly the radiative transfer equation in the spectral domain. When available data for the modelling are missing, approximate methods can palliate for the lack of global interpretation of some molecular bands. In the case of CH_4 in the giant planet spectra, it is of interest to note that this molecule still presents unexplored range, especially at short wavelengths. Indeed, the optical paths in planetary atmospheres at temperatures as low as 100 K reach kilometre-amagat (one amagat being the gas density at standard pressure and temperature), which is difficult, or even impossible to reach in laboratory. In such a case, models using average opacities over limited spectral intervals can be used, instead of individual lines (band models). The comparison in recovering regions with more exact models have allowed planetary scientists to estimate the accuracy of such models.

2.1.5. Data bases

The access to the molecular data is also an important face of the problem of the modelisation of planetary spectra, as spectroscopic measurements have to be safely compiled and stored in huge data banks. Most used data bases are HITRAN [9] or GEISA [10]. The question of data validation, and access to more specialized parameters is nevertheless endless.

2.2. Inversion methods

From the parameters described above, a direct calculation of planetary synthetic spectra can be reproduced. Such a calculation supposes the planetary structure well known: temperature profile, composition, cloud structure are the needed ingredients of the calculation. In any case, the main objective of spectral measurements is of course to retrieve these planetary parameters, and the modeller face a classical inversion problem. Different techniques are used to reach such measurements, with a common assumption (always to be verified) that the parameters have to be separable in their contribution to the spectrum. The simplest inversion method consists in creating a data base of synthetic spectra, including all the expected variations of all the parameters [11]. It remains to extract the measurement from a least square fit to an observed spectra, but many difficulties can arise from ambiguities inherently present in planetary spectra.

3. Planetary spectroscopy

Each planet has a single fingerprint, and raise specific questions to planetologists; nevertheless, general methods of spectral observation are similar from one planet to another. Fig. 3 shows spectra observed with the SWS instrument (Short Wavelength Spectrograph) of ISO satellite (Infrared Space Observatory from the European Space Agency) for the four giant planets [12,13]. An overview of the recovered physical parameters is the following.

3.1. Abundance measurements

The measure of chemical composition is one of the most traditional objectives of spectroscopy. The first outstanding successes in the determination of atmospheric composition are the detection of methane and ammonia in giant planet atmospheres [1], as well as methane on Titan in 1944 [14]. The importance of chemical composition on the physics of atmospheric planets is multiple:

- On Giant Planets, primordial mixing ratios of fundamental chemical elements are retrieved, in order to constrain the models of planetary formation and planetary evolution [15]. Measurements of H/He, C/H, N/H, O/H are among the most frequent retrievals. For these compounds, a comparison with the composition of the primitive solar nebula in heavy elements is searched, which for giant planets is related to the accretion processes with the formation of an ice/rock nucleus before gas accretion from the solar nebula. In the case of condensable species, like H_2O, such measurements are valid only if the deep abundance is retrieved below any condensable layer [16]. On Jupiter and for the most abundant minor species, it is true only for CH_4. Representative values of NH_3 or H_2O abundances from Voyager/IRIS spectral interpretation were only partially raised after the Galileo probe direct measurement in 1995 [17].
- On Venus [18], minor species retrieval in the deep atmosphere, like H_2O, CO, OCS give information on the thermochemical equilibrium state of the atmosphere, in equilibrium with the surface, which present high temperatures (about 450 °C).
- On Mars, composition variations are studied mostly for meteorological constraints [19], with H_2O variations related to the Martian meteorology: diurnal, seasonal and local variations are today predicted by global circulation models. Carbon monoxide is measured in millimetre waves and in the infrared, and its global distribution and variation is still discussed. Finally, the controversial detection by Mars Express of CH_4 in Martian atmosphere [20] is exemplar of the importance of spectroscopy to planetary exploration, even in the Martian space exploration era.

3.2. Isotopic ratios

Even if isotopic measurements are only a special case of abundance measurements, the specific problems they raise, both observational and interpretational, needs a specific discussion:

For instance, the D/H ratio [21] measured from CH_4/CH_3D is very different in giant planets than in comets (from H_2O/HDO), where a strong enrichment is observed, probably due to the interstellar ion chemistry on grains from which the comets are formed. The telluric planetary atmospheres exhibit intermediate values, coming from a 'cometary pollution' (Earth) or differential escape of H_2O compared to HDO (Venus). Isotopic ratios of nitrogen or oxygen raise different problems. In the case of variations from planet to planet, the invoked processes are either an intrinsic inhomogeneity of the primitive solar nebula, either fractionation processes inside the atmospheres. As an example, the $^{14}N/^{15}N$ ratio on Jupiter is very different from the Earth [22], the interpretation being still pending.

3.3. Thermal profiles

Planetary thermal profiles can be retrieved from planetary thermal emission in strong infrared bands. Although any constituent could, in principle, be used for such purposes, it is, of course, more efficient to use well known compounds, with uniform density distribution. On giant planets and Titan, CH_4 is commonly used, or CO_2 on Venus and Mars. The inversion of the temperature/pressure profile from the infrared spectra is one of the most common use of radiative transfer methods on Earth as on other planets, which is well documented in the literature [23].

3.4. Pressure measurements

When the spectrally active constituent is also a major element of the atmosphere, its abundance measurement on the ground is equivalent to a measure of the atmospheric pressure, which is the total weight of an atmospheric column over a square area. In the case of Mars, spectroscopic measurements have been used for such purpose [24]; since atmospheric pressure is related to the altitude of the surface, spectral measurements have provided an accurate relative altimetry, well before the measurement of Mars Global Surveyor laser altimeter.

3.5. Cloud structure measurements

Cloud structure has different effects on the planetary spectra: first, clouds act as a reflecting layer of the solar flux, and the pressure level of the cloud controls the column density of the measured constituents, in a simple reflecting layer model. Even such simple models of clouds give interesting results on the altitude variations of the clouds of Jupiter, for example.

More sophisticated models need to take into account the spectroscopy and the scattering mechanisms within the clouds [25]. Such models, although much more complex are today available; the principal limitation is not so much the computational time for direct models, than the difficulty to invert the parameters from the observations, as the large number of parameters preclude independent retrieval of each of them.

4. Conclusion

Spectroscopy remains in the era of planetary exploration of planetary atmospheres from Venus to Pluto an essential tool for the progress of our knowledge. Progress in spectroscopy, in parallel with instrumentation and planetary modelling, is essential to the planetology field, especially for atmospheric sounding. Even simple molecules like CH_4 have a still incomplete spectral database, especially at shorter wavelengths in the infrared, which limits the fine interpretation of spectra. Coordination between planetology and spectroscopy is one of the strongest hope for future advances in this domain.

References

[1] R. Wildt, Naturwiss. 20 (1932) 851.

[2] R.M. Goody, Y.L. Yung, Atmospheric Radiation: Theoretical Basis, second ed., Oxford Univ. Press, New York, 1989.

[3] G. Birnbaum, A. Borysow, G.S. Orton, Collision-induced absorption of H2–H2 and H2–He in the rotational and fundamental bands for planetary applications, Icarus 123 (1996) 4–22.

[4] D. Gautier, B. Conrath, M. Flasar, R. Hanel, V. Kunde, A. Chedin, N. Scott, The helium abundance of Jupiter from Voyager, J. Geophys. Res. 86 (1981) 8713.

[5] J.F. D'Eu, B. Lemoine, F. Rohart, Infrared HCN lineshapes as a test of Galatry and speed-dependent Voigt profiles, J. Mol. Spectrosc. 212 (2002) 96–110.

[6] D. Pieroni, T. Nguyen Van, C. Brodbeck, J.M. Hartmann, T. Gabard, J.P. Champion, D. Bermejo, J.L. Domenech, C. Claveau, A. Valentin, Experimental and theoretical study of line mixing in methane spectra. IV. Influence of the temperature and of the band, J. Chem. Phys. 113 (2000) 5776–5783.

[7] J.F. Appleby, CH4 nonlocal thermodynamic equilibrium in the atmospheres of the giant planets, Icarus 85 (1990) 355–379.

[8] D. Gautier, B. Bézard, A. Marten, J.-P. Baluteau, N. Scott, A. Chedin, V. Kunde, R. Hanel, The C/H ratio in Jupiter from the Voyager infrared investigation, Astrophys. J. 257 (1982) 901–912.

[9] L.S. Rothman, C.P. Rinsland , A. Goldman, S.T. Massie, D.P. Edwards, J.-M. Flaud, A. Perrin, C. Camy-Peyret, V. Dana, J.-Y. Mandin, J. Schroeder, A. McCann, R.R. Gamache, R.B. Wattson , K. Yoshino, K. Chance, K. Jucks, L.R. Brown, V. Nemtchinov, P. Varanasi, The HITRAN molecular spectroscopic database and HAWKS (HITRAN Atmospheric Workstation), JQSRT 60 (1996) 665–710.

[10] N. Husson, B. Bonnet, N.A. Scott, A. Chedin, Management and study of spectroscopic information—the GEISA program, J. Quant. Spectrosc. Radiat. Transfer 48 (1992) 509–518.

[11] M. Roos-Serote, P. Drossart, T. Encrenaz, E. Lellouch, R.W. Carlson, K.H. Baines, L. Kamp, R. Mehlman, G.S. Orton, S. Calcutt, P. Irwin, F.W. Taylor, A. Weir, Analysis of Jupiter North Equatorial Belt hot spots in the 4–5-μm range from Galileo/near-infrared mapping spectrometer observations: Measurements of cloud opacity and water, and ammonia, J. Geophys. Res. 103 (1998) 23023–23042.

[12] T. de Graauw, H. Feuchtgruber, B. Bezard, P. Drossart, T. Encrenaz, D.A. Beintema, M. Griffin, A. Heras, M. Kessler, K. Leech, E. Lellouch, P. Morris, P.R. Roelfsema, M. Roos-Serote, A. Salama, B. Vandenbussche, E.A. Valentijn, G.R. Davis, D.A. Naylor, First results of ISO-SWS observations of Saturn: detection of CO_2_, CH_3_C_2_H, C_4_H_2_ and tropospheric H_2_O, Astronomy and Astrophysics 321 (1997) L13–L16.

[13] T. Encrenaz, T. de Graauw, S. Schaeidt, E. Lellouch, H. Feuchtgruber, D.A. Beintema, B. Bezard, P. Drossart, M. Griffin, A. Heras, M. Kessler, K. Leech, P. Morris, P.R. Roelfsema, M. Roos-Serote, A. Salama, B. Vandenbussche, E.A. Valentijn, G.R. Davis, D.A. Naylor, First results of ISO-SWS observations of Jupiter, Astronomy and Astrophysics 315 (1996) L397–L400.

[14] G.P. Kuiper, Titan: a satellite with an atmosphere, Astrophys. J. 100 (1944) 378–383.

[15] K. Atreya, M.H. Wong, T.C. Owen, P.R. Mahaffy, H.B. Niemann, I. De Pater, P. Drossart, T. Encrenaz, A comparison of the atmospheres of Jupiter and Saturn: deep atmospheric composition, cloud structure, vertical mixing and origin, Planetary and Space Sci. 47 (1999) 1243–1262.

[16] M. Roos-Serote, A.R. Vasavada, L. Kamp, P. Drossart, P. Irwin, C. Nixon, R.W. Carlson, Proximate humid and dry regions in Jupiter's atmosphere indicate complex local meteorology, Nature 405 (2000) 158–160.

[17] H.B. Niemann, S.K. Atreya, G.R. Carignan, T.M. Donahue, J.A. Haberman, D.N. Harpold, R.E. Hartle, D.M. Hunten, W.T. Kasprzak, P.R. Mahaffy, T.C. Owen, S.H. Way, The composition of the Jovian atmosphere as determined by the Galileo probe mass spectrometer, J. Geophys. Res. 103 (1996) 22831–22846.

[18] B. Bézard, C. de Bergh, D. Crisp, J.P. Maillard, The deep atmosphere of Venus revealed by high resolution spectroscopy, Nature 356 (1990) 508–511.

[19] T. Encrenaz, The atmosphere of Mars as constrained by remote sensing, Space Sci. Rev. 96 (2001) 411–424.

[20] V. Formisano, S. Atreya, T. Encrenaz, N. Ignatiev, M. Giuranna, Detection of methane in the atmosphere of Mars, Science 306 (2004) 1758–1761.

[21] D. Gautier, M. Gerin, E. Roueff, Special issue on deuterium in the Universe, Planetary and Space Sci. 50 (2002) 1123–1123.

[22] T. Fouchet, P.G.J. Irwin, P. Parrish, S.B. Calcutt, F.W. Taylor, C.A. Nixon, T. Owen, Search for spatial variation in the Jovian $^{15}N/^{14}N$ ratio from Cassini/CIRS observations, Icarus 172 (2004) 50–58.

[23] D. Gautier, R. Courtin, Atmospheric thermal structures of the giant planets, Icarus 39 (1979) 28–45.

[24] E. Gendrin, S. Erard, P. Drossart, R. Melchiorri, Observation of pressure variations in the Martian atmosphere, Geophys. Res. Lett. 30 (2003) ASC14-1.

[25] P.G.J. Irwin, A.L. Weir, S.E. Smith, F.W. Taylor, A.L. Lambert, S.B. Calcutt, P.J. Cameron-Smith, R.W. Carlson, K.H. Baines, G.S. Orton, P. Drossart, T. Encrenaz, M. Roos-Serote, Cloud structure and atmospheric composition of Jupiter retrieved from Galileo near-infrared mapping spectrometer real-time spectra, J. Geophys. Res. 103 (1998) 23001–23022.