

Exploring extrasolar worlds: from gas giants to terrestrial habitable planets

Giovanna Tinetti,^{*a} Caitlin A. Griffith,^b Mark R. Swain,^c
Pieter Deroo,^c Jean Philippe Beaulieu,^{ad} Gautam Vasisht,^c
David Kipping,^{ae} Ingo Waldmann,^a Jonathan Tennyson,^a
Robert J. Barber,^a Jeroen Bouwman,^f Nicole Allard^d
and Linda R. Brown^c

Received 14th April 2010, Accepted 27th April 2010

DOI: 10.1039/c005126h

Almost 500 extrasolar planets have been found since the discovery of 51 Peg b by Mayor and Queloz in 1995. The traditional field of planetology has thus expanded its frontiers to include planetary environments not represented in our Solar System. We expect that in the next five years space missions (Corot, Kepler and GAIA) or ground-based detection techniques will both increase exponentially the number of new planets discovered and lower the present limit of a ~ 1.9 Earth-mass object [e.g. Mayor *et al.*, *Astron. Astrophys.*, 2009, **507**, 487]. While the search for an Earth-twin orbiting a Sun-twin has been one of the major goals pursued by the exoplanet community in the past years, the possibility of sounding the atmospheric composition and structure of an increasing sample of exoplanets with current telescopes has opened new opportunities, unthinkable just a few years ago. As a result, it is possible now not only to determine the orbital characteristics of the new bodies, but moreover to study the exotic environments that lie tens of parsecs away from us. The analysis of the starlight not intercepted by the thin atmospheric limb of its planetary companion (transit spectroscopy), or of the light emitted/reflected by the exoplanet itself, will guide our understanding of the atmospheres and the surfaces of these extrasolar worlds in the next few years. Preliminary results obtained by interpreting current atmospheric observations of transiting gas giants and Neptunes are presented. While the full characterisation of an Earth-twin might require a technological leap, our understanding of large terrestrial planets (so called super-Earths) orbiting bright, later-type stars is within reach by current space and ground telescopes.

1 Introduction

Half a century ago, the space age began with the launch of Sputnik. Now at the completion of a fairly detailed study of the planets of our own solar system, we are at the dawn of the age of exoplanets. Almost 500 exoplanets, *i.e.* planets orbiting a star different from our Sun, are now known thanks to indirect detection

^aDepartment of Physics and Astronomy, University College London, Gower Street, London, UK WC1 E6BT. E-mail: g.tinetti@ucl.ac.uk

^bLPL, University of Arizona, 1629 E. University Blvd, Tucson, AZ, 85721, USA

^cJet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA, 91109, USA

^dInstitut d'Astrophysique de Paris, 98bis Boulevard Arago, Paris, France

^eHarvard-Smithsonian Center for Astrophysics (CfA), 60 Garden Street, Cambridge, MA, 02144, USA

^fMax-Planck-Institut fuer Astronomie, Koenigstuhl 17, 69117 Heidelberg, Germany

techniques.¹ In the first decade after their initial discovery in 1995,² the task was to find more and more of these astronomical bodies: the biggest, the smallest; the hottest, the coolest; the system with the most planets in it. In recent years, attention has switched from finding planets to characterising them. Among the variety of exoplanets discovered so far, special attention has been devoted to those planets which transit their parent star, whose presence can be detected by the reduction in the brightness—the extinction—of the central star as the planet passes in front of it. More than 106 currently identified exoplanets are transiting planets, and for these objects planetary and orbital parameters such as radius, eccentricity, inclination, mass (given by radial velocity combined measurements), are known, allowing first order characterisation on the bulk composition and temperature (Gas giant? Neptune type? Terrestrial?). But it is clear that there is great variety even amongst the family of transiting exoplanets. The smallest, Corot-7b³ and GJ1214b,⁴ have masses of just 0.0151 and 0.0179 M_J . They orbit their parent star at distances of <0.02 AU. At the other end of the transiting planet distance scale, HD 80606 b orbits its G5 star with a period of more than 100 days and an eccentricity of 0.93. And at the high mass end, WASP-18b and XO-3b have a mass of 10.43 and 11.79 M_J and their atmospheric temperature is likely to be very hot.

Most importantly recent results have been able to demonstrate that for transiting exoplanets orbiting stars brighter than 12 Mag, it is possible to identify the main chemical components in the planet's atmosphere. A stellar occultation (called primary transit) occurs when the light from a star is partially blocked by an intervening body, such as a planet. With this method, we can indirectly observe the thin atmospheric ring surrounding the optically thick disk of the planet while the planet is transiting in front of its parent star.^{5,6} In the secondary transit technique, we firstly observe the combined spectrum of the star and the planet. Then, we take a second measurement of the star alone when the planet disappears behind it: the difference between the two measurements consists of the planet's own spectrum.^{7,8}

In the past 3 years, key observations with the Spitzer and Hubble Space Telescopes have, for the first time, given us real insights into the composition of some of the most unusual exoplanets so far discovered—the class known as hot-Jupiters. More specifically, infrared transmission and emission spectroscopy have revealed the presence of the primary carbon and oxygen species such as CH₄, CO₂, CO, and H₂O,^{9–16} and provided constraints for the temperature profiles,^{17–20} which are coupled to the composition. Today, broad-band or low-resolution spectroscopy from ground and space based observatories allow us to:

- determine planetary and orbital parameters
- constrain the albedo
- detect the main molecular species in the hot transiting planets' atmosphere
- constrain the horizontal and vertical thermal gradients in the hot exoplanets' atmospheres
 - constrain the boundary conditions in the upper atmosphere
 - detect the presence of clouds or hazes

Relatively high resolution spectroscopy data were recently obtained with ground-based telescopes in the optical^{21,22} and NIR,^{23,24a} confirming that alkali metals are present in hot-Jupiter atmospheres and showing non thermal emission processes. These achievements open up enormous possibilities in terms of atmospheric characterisation for the short term future prior to the launch of the next generation of space telescopes (the James Webb Space Telescope, launch 2014) or a dedicated mission (e.g. ECHO, the Exoplanet Characterization Observatory, <http://echo-spacemission.eu>).

With current instruments we can already study the atmospheres of more than ten transiting hot-Jupiters and approach the case of hot Neptunes and warm super-Earths transiting later type stars, e.g. GJ436 b and GJ1214 b. Surveys aimed at detecting extrasolar planets are focusing on searches for ever smaller worlds and rocky

planets in the habitable zones. While Corot and Kepler will increase the statistics of such objects with the ultimate goal of detecting earth-like planets around G-type stars, transit and radial velocity surveys from the ground (HARPS, MEarth, WFCAM Transit Survey) will actually provide the optimal targets for atmospheric characterisation, in particular super-Earths transiting bright M-dwarfs down to the habitable zone. Feasibility studies show that those objects will be easily studied by JWST and EChO-like missions.^{24b}

2 Retrieving atmospheric parameters from exoplanet spectra

Within the past year, efforts to determine the abundances of atmospheric constituents found instead a range of degenerate temperature and composition solutions from the spectra,^{16,20,26} see Fig. 1. Using an iterative forward model approach for spectral retrieval, we evaluated a variety of temperatures (T) as a function of pressure (P) together with the molecular absorption effects. Combining near-infrared spectra with mid-infrared measurements, we find that absorption due to H₂O, CH₄ and CO₂ explains most of the features present in the observed hot-Jupiter spectra (see Fig. 1). The additional contribution of CO is more than plausible and in few cases it even refines our fit, but we cannot discard the possibility that improved data lists for methane and/or CO₂ would provide the missing opacity. The radiative transfer calculations assume local thermal equilibrium (LTE) conditions—as expected for pressures exceeding 10⁻³ bar that are probed by the infrared spectra—and constant mixing ratios for the molecules.

For emission spectra, we obtain a family of plausible solutions for the molecular abundances and detailed temperature profiles for most of the hot-Jupiters observed. In Fig. 1 we show the example of HD 209458 b,²⁰ for which both NIR and MIR spectroscopical and photometrical data are available. Additional observational constraints on the atmospheric temperature structure and composition require either improved wavelength coverage/spectral resolution for the dayside spectrum or a transmission spectrum. The degeneracy is even higher when only a handful of photometrical observations are available (Fig. 2), calling for caution against premature theoretical classifications, such as the idea that hot-Jupiters may be divided in

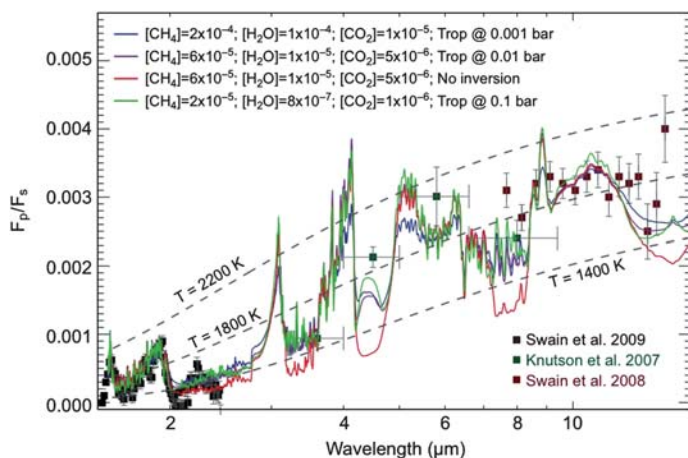


Fig. 1 Emission photometry and spectroscopy data for HD 209458 b.²⁰ The near-infrared and mid-infrared observations compared to synthetic spectra for four models that illustrate the range of temperature/composition possibilities consistent with the data. For each model case, the molecular abundance of CH₄, H₂O, & CO₂ and the location of the tropopause is given, these serve to illustrate how the combination of molecular opacities and the temperature structure cause significant departures from a purely single-temperature thermal emission spectrum.

two classes, where the presence or absence of a stratosphere is caused by the presence or absence of TiO/VO.²⁷

Transmission spectra are less sensitive to the atmospheric temperatures, yet the derived composition at the terminator depends sensitively on the assumed radius. In particular the atmospheric temperature may play an important role in the overall scale height, and hence in the amplitude of the spectral signatures, as well as in the molecular absorption coefficients. For most cases a thermochemical equilibrium H₂O abundance of 4.5×10^{-4} relative to H₂^{28–30} provide an excellent match to the data, see *e.g.* the case of XO-2b, Fig. 3. However, a $\sim 1\%$ difference in the estimate of the planetary radius at the ~ 1 bar pressure level, would result in a variation of the H₂O abundances by a factor of 10. Transit data at multiple wavelengths are needed to constrain the H₂O abundance. The mixing ratios determined for CH₄, CO and CO₂ depend on the data lists used and on the H₂O mixing ratio.

In Fig. 4 we consider the planet HD 189733 b. While most of the photometric and spectroscopic data are explainable with the presence of water vapour³¹ and methane,¹¹ the recent observation of the photometric point at 4.5 μm ³² suggests

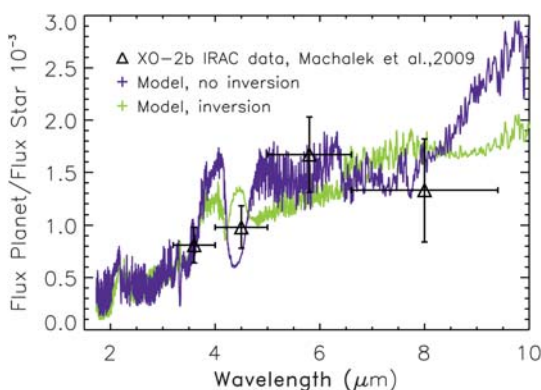


Fig. 2 Photometry secondary transit data obtained with the Spitzer IRAC instrument for the hot-Jupiters XO- 2b.²⁵ In color are overlotted the atmospheric models for XO-2b containing water, methane, CO and CO₂. Blue line: simulated spectrum of XO-2b obtained using a T - P profile with no temperature inversion. Green line: simulated spectrum of XO-2b obtained using a T - P profile with temperature inversion.

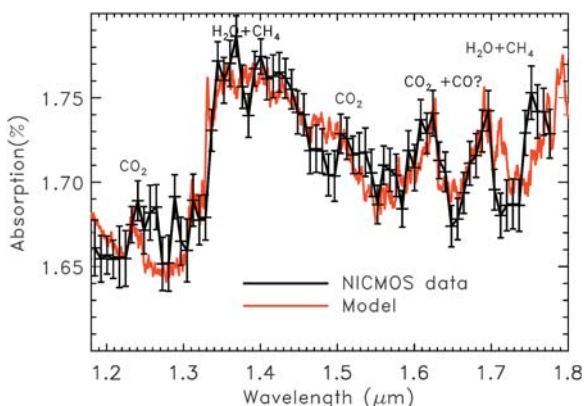


Fig. 3 Transmission spectrum of the hot-Jupiter XO-1b,¹⁶ the fit was obtained with H₂O, CH₄, CO₂ and CO.

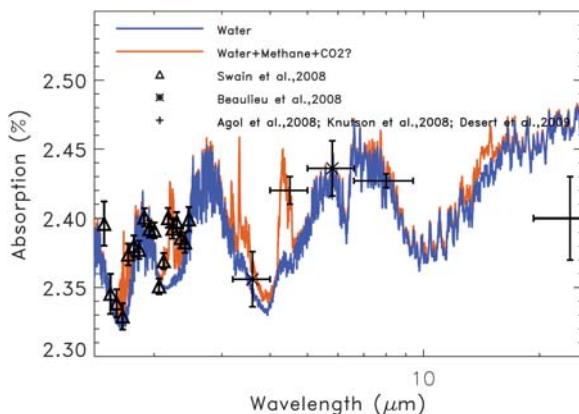


Fig. 4 Primary transit photometry and spectroscopy data of HD 189733 b recorded by multiple instruments and different teams. While most of the features can be explained by a combination of water vapour and methane, the IRAC band at 4.5 μm seems to indicate the additional presence of CO_2 and/or CO.

the additional presence of CO_2 and possibly CO in that planetary atmosphere. The addition of a small quantity of CO_2 and CO does not affect the fit at shorter wavelengths, and has the advantage of being consistent with the “day-side” composition observed with NICMOS.¹³ We note that some of the temperature profiles/molecular mixing ratios consistent with the observations raise the question of whether the dayside atmosphere is in radiative and thermochemical equilibrium. Although advection of heat and/or photochemistry could support departures from radiative and thermochemical equilibrium (Fig. 5), our present lack of knowledge of molecular opacities at high temperatures for species such as CH_4 , H_2S and C_2H_6 limits our ability to determine decisively whether this condition is met or not; thus there is an urgent need for further laboratory studies to obtain molecular databases for determining high temperature opacities of the most common molecules expected in hot-Jupiter/hot-Neptune atmospheres.

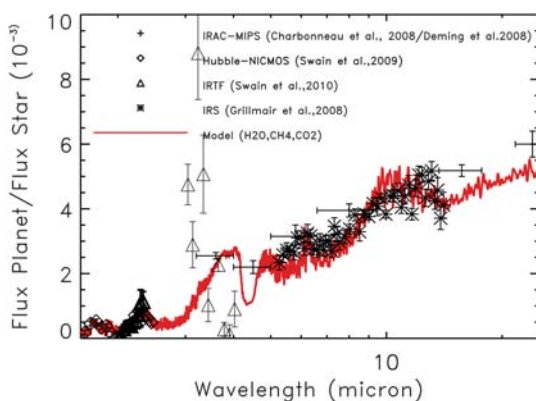


Fig. 5 Emission photometry and spectroscopy data for HD 189733 b. A radiative transfer model (red) assuming LTE conditions and consistent with the measurements made with Spitzer and Hubble fails to describe the emission structure at 3.1–4.1 μm ,²³ and we find no plausible combination of atmospheric parameters that provides a good model of the observations under LTE conditions. The brightness temperature of the 3.25 μm emission feature indicates the likely presence of a non-LTE emission mechanism.

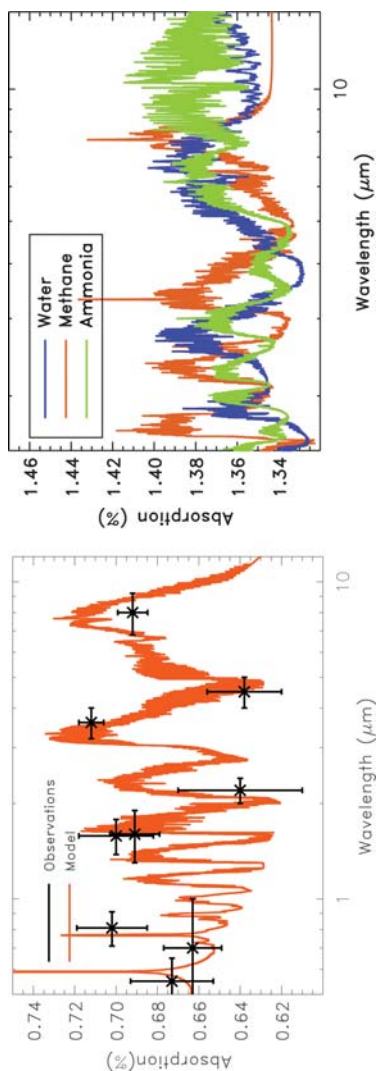


Fig. 6 Simulated transmission spectrum for the hot-Neptune GJ 436 b and the warm super-earth GJ 1214 b. The models contain molecular hydrogen, methane, water vapour and ammonia. GJ 1214 b atmosphere is here supposed to contain mainly molecular hydrogen and that is why the molecular features are very prominent. If the main component of its atmosphere is a heavier molecule, then the spectral features will be far less detectable. Observations will soon be available to confirm or reject the theoretical predictions.

We show in (Fig. 6) simulated transmission spectra for the hot-Neptune GJ436 b and the warm super-Earth GJ1214 b in the case its very extended atmosphere is mainly composed of molecular hydrogen. The spectral features in both cases are measurable with current space and ground-based observatories and more observations will probably become available in the next months.

3 The models

We model the transmission and emission spectra of transiting exoplanets using line-by-line radiative transfer models which account for the effects of molecular opacities^{9,31,33} and hazes.^{34,35} In our simulations we include H₂–H₂, H₂O, CH₄, CO, CO₂, NH₃, HCN *etc.* While the BT2 line list for water³⁶ can be calculated at the appropriate temperatures, the available data lists for methane at high temperature are inadequate to probe the modulations of the atmospheric thermal profile. To cover the spectral range from the visible to the Mid-IR, we have to use multiple data lists for methane, HITRAN 2008, PNNL, and hot-temperature measurements at 800, 1000 and 1273 K.³⁷ The Nassar and Bernath³⁷ data provide a much better fit to our observations in the region where they overlap with HITRAN 2008.³⁸ Compared to the results obtained with the Nassar and Bernath³⁷ line lists, mixing ratios 10–50 times larger are needed for methane if we use PNNL³⁹ or HITRAN 2008. The HITRAN 2008 data bank has the advantage of covering the entire spectral range measured by Hubble and Spitzer, with the downside (shared also by the PNNL list) that it results from measurements at room temperature, and therefore is quite inadequate to estimate the mixing ratio of methane at the temperatures of interest for hot planets. For CO₂ we use HITEMP⁴⁰ and CDSD-1000,⁴¹ for CO we also use HITEMP. The contribution of H₂–H₂ at high temperatures was taken from ref. 42. The opacity was interpolated to the temperature of each atmospheric layer. As collision induced absorption scales with the square of the pressure, the H₂–H₂ contribution becomes important for pressures higher than 1 bar. The line shapes of alkali metals are calculated at different temperatures and interpolated for intermediate values. Their spectral contribution becomes important in the visible-NIR wavelength range.⁴³ An accurate line list for ammonia at has recently been calculated⁴⁴ and its extension to high temperatures achieved.⁴⁵

4 Conclusions

An aspect of exoplanetary science that is both high-impact and cutting-edge is the study of extrasolar planet atmospheres. The ultimate goal is to obtain a high-resolution spectrum of an Earth-like planet, and although such a goal remains lofty, the key intermediate steps towards this end are already being taken with current technology for planets which are more massive and/or warmer than our own Earth. The characterisation of exoplanet atmospheres with current telescopes can be tackled with two main approaches: low resolution spectroscopy, from space using SPITZER and HST or the ground (*e.g.* NASA-IRTF), and high resolution spectroscopy from the ground (for example, VLT CRIRES). We can already probe the atmospheric constituents of several giant exoplanets, which orbit very close to their parent star, using transit techniques. The observations can be explained mainly with the combined presence of H₂O, CH₄, CO and CO₂ in the atmosphere of the planet. The photometric and spectroscopic emission data observed are consistent with the above composition but a variety of *T–P* profiles and mixing ratios are compatible with the data. Additional observations of transiting hot-Jupiters, especially spectroscopic data, will allow a more thorough classification of this type of planets unknown in our Solar System.

With current telescopes we can also approach the case of hot Neptunes and large terrestrial planets (super-Earths) transiting bright later type stars, *e.g.* GJ 436b or GJ 1214 b. Thanks to Corot, Kepler, ground-based transit surveys and the

improvements in radial velocity measurements, many rocky planets and [possible Online](#) few exomoons, are expected to be discovered in the next months/years. Further into the future, the James Webb Space Telescope will be the next generation of space telescopes to be online (launch 2014) and a dedicated mission to characterise transiting exoplanet atmospheres has been recently being proposed to NASA and ESA (EChO). Those observatories will guarantee high spectral resolution from space and the characterisation of smaller/colder targets, allowing us to expand the variety of characterisable extrasolar planets down to terrestrial planets and/or habitable zone of stars cooler than the Sun.

Acknowledgements

G. T. is supported by a Royal Society University Research Fellowship. Part of the research at the Jet Propulsion Laboratory (JPL), California Institute of Technology, was performed under contracts and grants with National Aeronautics and Space Administration.

References

- 1 J. Schneider, <http://www.exoplanet.eu>, 2010.
- 2 M. Mayor and D. Queloz, *Nature*, 1995, **378**, 355.
- 3 A. Leger, D. Rouan, J. Schneider, P. Barge, M. Fridlund, B. Samuel, M. Ollivier, E. Guenther, M. Deleuil, H. Deeg, M. Auvergne, R. Alonso, S. Aigrain, A. Alapini, J. Almenara, A. Baglin, M. Barbieri, H. Bruntt, P. Borde, F. Bouchy, J. Cabrera, C. Catala, L. Carone, S. Carpano, S. Csizmadia, R. Dvorak, A. Erikson, S. Ferraz-Mello, B. Foing, F. Fressin, D. Gandolfi, M. Gillon, P. Gondoin, O. Grasset, T. Guillot, A. Hatzes, G. Hebrard, L. Jorda, H. Lammer, A. Llebaria, B. Loeillet, M. Mayor, T. Mazeh, C. Moutou, M. Paetzold, F. Pont, D. Queloz, H. Rauer, S. Renner, R. Samadi, A. Shporer, C. Sotin, B. Tingley and G. Wuchterl, *Astron. Astrophys.*, 2009, **506**, 287.
- 4 D. Charbonneau, Z. K. Berta, J. Irwin, C. J. Burke, P. Nutzman, L. A. Buchhave, C. Lovis, X. Bonfils, D. W. Latham, S. Udry, R. A. Murray-Clay, M. J. Holman, E. E. Falco, J. N. Winn, D. Queloz, F. Pepe, M. Mayor, X. Delfosse and T. Forveille, *Nature*, 2009, **462**, 891–894.
- 5 T. M. Brown, *Astrophys. J.*, 2001, **553**, 1006.
- 6 D. Charbonneau, T. M. Brown, R. W. Noyes and R. L. Gilliland, *Astrophys. J.*, 2002, **568**, 377.
- 7 D. Deming, S. Seager, L. J. Richardson and J. Harrington, *Nature*, 2005, **434**, 740.
- 8 D. Charbonneau, L. E. Allen, S. T. Megeath, G. Torres, R. Alonso, T. M. Brown, R. L. Gilliland, D. W. Latham, G. Mandushev and F. T. O. nad Alessandro Sozzetti, *Astrophys. J.*, 2005, **626**, 523.
- 9 G. Tinetti, M. C. Liang, A. Vidal-Madjar, D. Ehrenreich, A. L. des Etangs and Y. Yung, *Astrophys. J.*, 2007, **654**, L99.
- 10 T. Barman, *Astrophys. J.*, 2008, **676**, L61.
- 11 M. R. Swain, G. Vasisht and G. Tinetti, *Nature*, 2008, **452**, 329.
- 12 C. J. Grillmair, A. Burrows, D. Charbonneau, L. Armus, J. Stauffer, V. Meadows, J. van Cleve, K. von Braun and D. Levine, *Nature*, 2008, **456**, 767.
- 13 M. Swain, G. Vasisht, G. Tinetti, J. Bouwman, P. Chen, Y. Yung, D. Deming and P. Deroo, *Astrophys. J.*, 2009, **690**, L114.
- 14 J. P. Beaulieu, S. Carey, I. Ribas and G. Tinetti, *Astrophys. J.*, 2008, **677**, 1343.
- 15 J. Beaulieu, D. Kipping, V. Batista, G. Tinetti, I. Ribas, S. Carey, J. A. Noriega-Crespo, C. A. Griffith, G. Campanella, S. Dong, J. Tennyson, R. Barber, P. Deroo, S. Fossey, D. Liang, M. R. Swain, Y. Yung and N. Allard, *Mon. Not. R. Astron. Soc.*, 2010 DOI: [astroph 0909.0185](https://doi.org/10.1093/mnras/stt185).
- 16 G. Tinetti, P. Deroo, M. R. Swain, C. A. Griffith, G. Vasisht, L. R. Brown, C. Burke and P. McCullough, *Astrophys. J.*, 2010, **712**, L139.
- 17 J. Harrington, B. M. Hansen, S. H. Luszcz, S. Seager, D. Deming, K. Menou, J. Cho and L. J. Richardson, *Science*, 2006, **314**, 623.
- 18 H. A. Knutson, D. Charbonneau, L. E. Allen, J. J. Fortney, E. Agol, N. B. Cowan, A. P. Showman, C. S. Cooper and S. T. Megeath, *Nature*, 2007, **447**, 183.
- 19 A. Burrows, J. Budaj and I. Hubeny, *Astrophys. J.*, 2007, **668**, L171.

- 20 M. Swain, G. Tinetti, G. Vasisht, P. Deroo, C. Griffith, J. Bouwman, P. Chen, A. Burrows, L. Brown, J. Matthews, J. Roe, R. Kuschnig and D. Angerhausen, *Astrophys. J.*, 2009, **704**, 1616.
- 21 S. Redfield, M. Endl, W. Cochran and L. Koesterke, *Astrophys. J.*, 2008, **673**, L87.
- 22 I. Snellen, S. Albrecht, E. de Mooij and R. L. Poole, *Astron. Astrophys.*, 2008, **487**, 357.
- 23 M. R. Swain, P. Deroo, C. A. Griffith, G. Tinetti, A. Thatte, G. V. P. Chen, J. Bouwman, I. J. Crossfield, D. Angerhausen, C. Afonso and T. Henning, *Nature*, 2010, **463**, 637.
- 24 (a) I. Snellen, R. de Kok, E. de Mooij and S. Albrecht, The orbital motion, absolute mass and high-altitude winds of HD 209458b, *Nature*, 2010, **465**, 1049; (b) Tessenyi *et al.*, submitted.
- 25 P. Machalek, P. R. McCullough, A. Burrows, C. J. Burke, J. L. Hora and C. M. Johns-Krull, *Astrophys. J.*, 2009, **701**, 514.
- 26 N. Madhusudhan and S. Seager, *Astrophys. J.*, 2009, **707**, 24.
- 27 J. J. Fortney, K. Lodders, M. S. Marley and R. S. Freedman, *Astrophys. J.*, 2008, **678**, 1419.
- 28 M.-C. Liang, C. D. Parkinson, A. Y. Lee, Y. L. Yung and S. Seager, *Astrophys. J.*, 2003, **596**, L247.
- 29 M.-C. Liang, S. Seager, C. D. Parkinson, A. Y. Lee and Y. L. Yung, *Astrophys. J.*, 2004, **605**, L61.
- 30 K. Zahnle, M. Marley, R. Freedman, K. Lodders and J. Fortney, *Astrophys. J.*, 2009, **701**, L20.
- 31 G. Tinetti, A. Vidal-Madjar, M.-C. Liang, J.-P. Beaulieu, Y. Yung, S. Carey, R. J. Barber, J. Tennyson, I. Ribas, N. Allard, G. E. Ballester, D. K. Sing and F. Selsis, *Nature*, 2007, **448**, 169.
- 32 J.-M. Desert, A. L. des Etangs, G. Hebrard, D. K. Sing, D. Ehrenreich, R. Ferlet and A. Vidal-Madjar, *Astrophys. J.*, 2009, **699**, 478.
- 33 G. Tinetti, V. S. Meadows, D. Crisp, W. Fong, T. Velusamy and H. Snively, *Astrobiology*, 2005, **5**(4), 461.
- 34 C. A. Griffith, R. V. Yelle and M. S. Marley, *Science*, 1998, **282**, 2063.
- 35 C. A. Griffith, T. Owen and R. Wagener, *Icarus*, 1991, **93**, 362.
- 36 R. J. Barber, J. Tennyson, G. J. Harris and R. N. Tolchenov, *Mon. Not. R. Astron. Soc.*, 2006, **368**, 1087.
- 37 R. Nassar and P. Bernath, *J. Quant. Spectrosc. Radiat. Transfer*, 2003, **82**, 279.
- 38 L. Rothman, I. Gordon, A. Barbe, D. Benner, P. Bernath, M. Birk, V. Boudon, L. Brown, A. Campargue, J. Champion, K. Chance, L. Coudert, V. Dana, V. Devi, S. Fally, J. Flaud, R. Gamache, A. Goldman, D. Jacquemart, I. Kleiner, N. Lacome, W. Lafferty, J. Mandin, S. Massie, S. Mikhailenko, C. Miller, N. Moazzen-Ahmadi, O. Naumenko, A. Nikitin, J. Orphal, V. Perevalov, A. Perrin, A. Predoi-Cross, C. Rinsland, M. Rotger, M. Simeckova, M. Smith, K. Sung, S. Tashkun, J. Tennyson, R. Toth, A. Vandaele and J. V. Auwera, *J. Quant. Spectrosc. Radiat. Transfer*, 2009, **110**, 533.
- 39 PNNL, <http://www.pnl.gov/>.
- 40 L. S. Rothman, I. E. Gordon, R. J. Barber, H. Dothe, R. R. Gamache, A. Goldman, V. I. Perevalov, S. A. Tashkun and J. Tennyson, *J. Quant. Spectrosc. Radiat. Transfer*, 2010, **111**, 2139–2150.
- 41 S. A. Tashkun, V. Perevalov, J. Teffo, A. D. Bykov and N. N. Lavrentieva, *J. Quant. Spectrosc. Radiat. Transfer*, 2003, **82**, 165.
- 42 A. Borysow, U. G. Jorgensen and Y. Fu, *J. Quant. Spectrosc. Radiat. Transfer*, 2001, **68**, 235.
- 43 N. F. Allard, F. Allard, P. H. Hauschildt, J. F. Kielkopf and L. Machin, *Astron. Astrophys.*, 2003, **411**, L473.
- 44 S. N. Yurchenko, R. J. Barber, A. Yachmenev, W. Theil, P. Jensen and J. Tennyson, *J. Phys. Chem. A*, 2009, **113**, 11845–11855.
- 45 S. N. Yurchenko, R. J. Barber and J. Tennyson, *Mon. Not. R. Astron. Soc.*, 2010, submitted.