EXCELLENCE IN SCIENCE

THE ROYAL SOCIETY

THEO MURPHY INTERNATIONAL SCIENTIFIC MEETING ON

Water in the gas phase

Monday 13 – Tuesday 14 June 2011
The Kavli Royal Society International Centre

Organised by Professor Jonathan Tennyson FRS, Professor Keith Shine FRS, Professor Ewine van Dishoeck, Professor Peter Bernath and Dr Jonathan Taylor

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The abstracts that follow are provided by the presenters and the Royal Society takes no responsibility for their content.

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Water in the gas phase

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Synopsis
Water vapour's interaction with light is fundamental to understanding the Earth's climate, extrasolar planets (including attempts to detect life) and the chemistry of the interstellar medium. The discussion meeting will focus on fundamental developments in the spectroscopy of water, including its continuum, its role in the Earth's energy budget, and latest astronomical observations, including those from the Herschel space telescope

Monday 13 June 2011

9.00 Welcome by Professor Sir Peter Knight, Principal of Kavli Royal Society International Centre
Welcome by Professor Jonathan Tennyson, organiser

Session 1: Laboratory studies: fundamental
Chair – Professor Peter Bernath, University of York, UK

9.15 State-resolved spectroscopy of high vibrational levels of water up to the dissociative continuum
Dr Pavlo Maksyutenko, Paul Scherrer Institute, Switzerland

We summarize the experimental studies of high rovibronic energy levels of water molecules performed in the Laboratory of Molecular Physical Chemistry at EPFL, Switzerland. The use of double-resonance vibrational overtone excitation followed by energy selective photofragmentation and laser-induced fluorescence detection of OH fragments allowed us to measure the previously inaccessible rovibrational energies above the 7th OH stretch overtone. Extension of the experimental approach to triple-resonance excitation provided access to rovibronic levels through the transitions with significant transition dipole moments (mainly OH-stretch overtones) up to the dissociation threshold of the O-H bond. Collisionally assisted excitation schemes enabled us to probe vibrations that were not readily accessible via pure laser excitation. Observation of the continuous absorption onset yielded a very precise value for the O-H bond dissociation threshold, 41145.94 ± 0.15 cm-1. We detected long-lived resonances as sharp peaks in the spectra above the dissociation threshold.

9.45 Discussion

10.00 Global spectroscopy of the water monomer
Dr Oleg L Polyansky, Russian Academy of Sciences, Russia

Given the large energy required for electronic excitation, most important properties of the water monomer rely on its ground electronic state. Experiments are now probing the potential energy surface (PES) of this state over a very extended energy range. Progress in both characterising this surface and in analysing these experiments is described.

The water PES has been determined up to and beyond dissociation by combined *ab initio* and semi-empirical studies. As a first step, a very accurate, global, *ab initio* PES was determined using all-electron, internally-contracted multi-reference configuration interaction (IC-MRCI) and the aug-cc-pCV6Z basis set. Scalar-relativistic corrections were included. IC-MRCI energies were computed for a large set of about 2500 geometries, covering configurations from equilibrium up to dissociation.

Nuclear-motion calculations using this PES reproduce the observed energy levels up to 39 000 $cm^{-}1$ with an accuracy of better than 10 $cm^{-}1$. Line positions and widths of resonant states above dissociation show an agreement with experiment of about 50 $cm^{-}1$. The qualitative agreement between theoretical simulations and experimental spectra above dissociation is demonstrated in detail. An improved semi-empirical PES is produced by fitting the *ab initio* PES to accurate experimental data resulting in greatly improved accuracy of about 1 $cm^{-}1$.

Theoretical results based on the semi-empirical surface are compared with experimental data for energies starting at 27 000 $cm^{-}1$, going all the way up to dissociation at 41 000 $cm^{-}1$ and a few hundreds of wavenumbers beyond it (Ref.[1-3]). The study of the near-dissociation spectrum is based on an analysis of the conventional water spectra up to 26 000 $cm^{-}1$; a brief overview of this approach and of its connection to dissociation studies is given.

A new, extremely accurate, global, dipole moment surface for water has also been produced using *ab initio* methods. Together with the use of the PES mentioned above this allowed the calculation of water Stark coefficients up to dissociation.

10.30 Discussion

10.45 Coffee

11.15 Spectroscopic measurement of the vapour pressure of ice

Dr Joseph Hodges, National Institute of Standards and Technology, USA

We present a laser absorption technique to measure the saturation vapour pressure of hexagonal ice. This method is referenced to the triple point state of water and uses frequency-stabilized cavity ring-down spectroscopy to probe four rotation-vibration transitions of $H_2{}^{16}O$ at wave numbers near 7180 cm^{-1}. Laser measurements are made at the output of a temperature-regulated standard humidity generator which contains ice. The dynamic range of the technique is extended by measuring the relative intensities of three weak/strong transition pairs at fixed ice temperature and humidity concentration. Our results agree with Wexler's ice vapour pressure correlation [A. Wexler, J. Res. NBS 81A, 5 (1977)] over the temperature range $0^{\circ}C$ to $-70^{\circ}C$ to within 0.5%.

11.45 Discussion

12.00 Collisional effects on H_2O absorption spectra

Dr Jean-Michel Hartmann, Université Paris, France

I will present a short review on the effects of inter-molecular collisions on the shape of (collisionally) isolated infrared lines of water vapour. It will be based on experimental and theoretical results obtained, in the last five years, in our group and thanks to collaborations with experimentalists (D Bermejo et al, M Birk et al) and theoreticians (R R Gamache et al, P Joubert et al) of other groups.

In the first part of my talk, I will focus on the basic collisional quantities that are the pressure-broadening and –shifting coefficients, central parameters of the Lorentzian profile and thus of any line-shape model. Through comparisons of measured values with calculations with a semi-classical model, the influence of the molecular states involved and of the temperature will be analyzed. In particular the influence of vibration on the broadening and shifting will be demonstrated together with the quite unusual fact that, for some lines, the broadening coefficient in cm^{-1}/atm increased with increasing temperature.

In the second part of my presentation, line shapes beyond the usual Voigt model will be considered by including "velocity effects". These include both the influence of collisionally induced velocity changes that lead to the so-called Dicke narrowing and that of the dependence of collisional parameters on the speed of the radiating molecule. Experimental evidence of deviations from the Voigt shape will be presented and analyzed with a model, for the velocity collision kernels, based on the Keilson and Storer approach. The interest of classical molecular dynamics simulations together with semi-classical calculations of the collisional parameters for line shape predictions from "first principles" will be discussed.

12.30 Discussion

13.00 Lunch

Session 2: The water vapour continuum in the Earth's atmosphere
Chair – Professor Jonathan Taylor, University College London, UK

14.00 Determination of water vapour continuum absorption coefficients from recent observations
Dr Eli Mlawer, Atmospheric and Environmental Research, Inc, USA

Water vapour continuum absorption is an important contributor to the earth's radiative cooling and energy balance. Here we describe the development and status of the MT_CKD water vapour continuum absorption model. The perspective adopted in developing the MT_CKD model has been to constrain the model so that it is consistent with quality analyses of spectral atmospheric measurements. Laboratory measurements are also considered. Keeping the model consistent with current observational studies necessitates periodic (typically once per year) updates to the water vapour continuum coefficients. Continuum coefficients in spectral regions that have not been subject to compelling analyses are determined by a mathematical formulation of the spectral shape associated with each water vapour monomer line. This formulation, based on spectral regions in which the coefficients are known with low uncertainties, is applied consistently to all water vapour lines from the microwave to the visible, and the results summed (separately for the self and foreign) to obtain continuum coefficients from 0-20,000 cm-1.

In addition to providing background on the MT_CKD formulation, we describe two recent updates. These include the adjustments in the far-infrared region (Delamere et al, 2010) due to ground-based measurements taken as part of the RHUBC-I campaign, as well as a recent analysis of self continuum absorption at 4 microns based on satellite- and ground-based observations.

14.30 Discussion

14.45 Measurements of the atmospheric water vapour continuum using a solar-pointing Fourier Transform Spectrometer
Dr Tom Gardiner, National Physical Laboratory, UK

Solar-pointing Fourier Transform Infrared (FTIR) Spectroscopy offers the capability to measure both the fine scale and broad band spectral structure of atmospheric transmission simultaneously across wide spectral regions. It is therefore potentially suited to the study of continuum absorption behaviour. However, in order to properly address this issue it is necessary to radiatively calibrate the FTIR instrument response.

A solar-pointing high-resolution FTIR spectrometer was deployed as part of the 'Continuum Absorption by Visible and Infrared radiation and its Atmospheric Relevance' (CAVIAR) consortium project at two field sites – a low altitude location at the UK Met Office base at Camborne, Cornwall, and a high altitude site at the International Scientific Station at the Jungfraujoch, Switzerland. The talk will describe the measurements made at these sites and the radiative calibration activity using an Ultra-High Temperature Blackbody and the many related influence factors. The on-going analyses of the results from the campaigns will be discussed in terms of comparisons to the latest laboratory studies of the monomer and continuum water vapour absorption.

15.15 Discussion

15.30 Tea

16.00 Airborne and satellite remote of the water vapour continuum in the far-IR spectral region
Dr Stuart Newman, Met Office, UK

Remote sensing of the atmosphere from space plays an increasingly important role in weather forecasting. Exploiting observations from the latest generation of weather satellites relies on an accurate knowledge of fundamental spectroscopy, including the water vapour continuum absorption. Field campaigns involving the Facility for Airborne Atmospheric Measurements (FAAM) research aircraft have collected a comprehensive data set, comprising remotely-sensed infrared radiance observations co-located with accurate measurements of the temperature and humidity structure of the atmosphere. These field measurements have been used to constrain the strength of the infrared water vapour continuum, in comparison with the latest laboratory and theoretical studies. The impact of these results on the remote sensing of water vapour from space is discussed.

17.15 Discussion

17.30 Poster Session

18.00 End of meeting

18.30 Drinks reception

18.45 Dinner

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Session 3: The water vapour continnum: theory and laboratory measurements
Chair – Dr Andrei Vigasin, Russian Academy of Sciences, Russia

9.00 Towards a new model of the water vapour continuum
Dr Igor V Ptashnik, University of Reading, UK, and Zuev Institute of Atmospheric Optics RAS, Russia

The nature of the water vapour continuum absorption and the possible contribution from water dimers (WD) has been debated for many years. Until recently the large difficulties in identifying WD absorption in atmospheric or in equilibrium laboratory conditions at ambient temperature, together with the absence of sufficiently reliable calculations of WD spectra, made it impossible to unambiguously resolve this debate. The rapidly growing possibilities in both spectroscopic experiments and theoretical quantum chemistry during the past decade or so have given second wind to this old debate. Detailed comparison of the modern measurements and ab initio predictions has revealed strong evidence for a dominant WD contribution to the continuum within near-infrared water vapour bands. Moreover, comparison of experimental data with the results of statistical partitioning of the pair states in phase space suggests that in many spectral regions bound and quasibound dimers may both contribute to spectral features of the water self-continuum at ambient temperature and pressure. This talk presents an analysis of retrievals of the continuum absorption in the whole near-infrared spectral region from recent laboratory measurements, which reveals some strong deviations from the modern commonly-used continuum models notably in window regions.

9.30 Discussion

9.45 The water-vapour continuum absorption in the mid-infrared10 and 4 µm atmospheric windows
Dr Yury Baranov, Institute of Experimental Meteorology, Russia

The pure water-vapour and water-nitrogen continuum absorption in the 10 and 4 µm atmospheric windows have been studied using a 2 m base-length White-type multipass cell coupled to a BOMEM DA3-002 FTIR spectrometer. The measurements were carried out at NIST over several years (2004-2007, 2009). New data on the $H_2O:N_2$ continuum in the 10 µm window are presented and summarized along with the other experimental results and the continuum model. The experimental data reported on the water-vapour continuum in the 10 and 4 µm atmospheric windows basically agree with the most reliable laboratory data from the other sources. One exception is the water-vapour self-continuum in the 4 µm spectral region, where our results strongly deviate from the measurements of Burch.

The MT_CKD continuum model significantly departs from the experimental data in both the 10 and 4 µm atmospheric windows. The observed deviation includes the continuum magnitude, spectral behaviour and temperature dependence. In the 4 µm region the model does not allow for the nitrogen fundamental collision induced absorption (CIA) band intensity enhancement caused by $H_2O:N_2$

collisions and strongly underestimates the actual absorption over two orders of magnitude. The water-vapour continuum interpretation as a typical CIA spectrum is reviewed and discussed.

10.15 Discussion

10.30 Coffee

11.00 IR shifts of the water dimer from the fully exible *ab initio* HBB2 potential
Professor Claude Leforestier, Université Montpellier, France

We report the calculations of the IR shifts for the water dimer, as obtained from the recent *ab initio* fully exible HBB2 potential energy surface of Bowman and co-workers. This potential was calculated at the [CCSD(T)] level, using the aug-cc-pVTZ basis set, and fitted to 30,000 distorted geometries. The rovibrational calculations, which formally are twelve-dimensional plus overall rotation, were performed within the [6 + 6]*d* adiabatic separation which decouples the "fast" intramolecular modes from the "slow" intermolecular ones. Apart from this decoupling, each set of modes is treated in a fully variational approach. The intramolecular motion was described in terms of Radau coordinates, using the f-embedding formulation of Wei and Carrington, and neglecting the rovibrational Coriolis coupling terms. Within this adiabatic approximation, the intermolecular motion is handled in a similar way as for rigid monomers, except for the rotational constants *B*'s, averaged over intramolecular modes, which depend now on the intermolecular geometry. Comparison to experimental data shows an excellent overall agreement, the large donnor bound $O\text{-}H_b$ IR shift (associated to the hydrogen bond) being however slightly off by ca. 12 cm^{-1}.

11.30 Discussion

11.45 Emerging measurement techniques
Discussion sessions led by Dr Rod Jones, University of Cambridge, UK

12.30 Lunch

Session 4: Astrophysics
Chair – Dr Steve Ball, University of Leicester, UK

13.30 The role of water vapour in the atmospheres of very low mass stars, brown dwarfs, and extrasolar planets
Dr France Allard, Centre de Recherche Astrophysique de Lyon, France

Since infrared observations of M dwarf stars (late 80's), brown dwarfs (mid 90's), and extrasolar planets (mid 2000s) are available, one of the most important challenge in modelling their atmospheres as become the understanding of water vapour formation. Model atmospheres and synthetic spectra (Allard PhDT '90, Allard & Hauschildt '95, Hauschildt, Allard & Baron '99, Allard et al '01) based on water vapour opacities evolving thought the years (Hot flames experiments by Ludwig 1972, Jorgensen et al '94, Miller & Tennyson '94, Schwenke et al 2002) have failed to reproduce the relative strength and shapes on the water bands clearly seen and shaping the low resolution ($R \leq 300$) infrared SEDs of M dwarfs. Yet the complexity of these atmospheres was only beginning to reveal itself.

Indeed, as ever lower mass and cooler objects were discovered thanks to the fantastic technologic development, it was shown that their spectral properties were affected by the greenhouse effects of dust cloud formation. Oxygen-rich dust grains (silicates) deplete as much as 20% of the oxygen content of the gas.

To understand this mechanism, we have developed radiation hydrodynamic 2D model atmosphere simulations to study the formation of forsterite dust in presence of hydrodynamical advection, condensation, and sedimentation across the M-L-T VLMs to BDs sequence (Teff=2800K to 900K, Freytag et al 2010). We discovered the formation of gravity waves as a driving mechanism for the formation of clouds in these atmospheres, and derived a rule for the velocity field versus atmospheric depth and Teff, which is relatively insensitive to gravity. This rule has been used in the construction of the new model atmosphere grid BT-Settl (Allard et al 2011, in preparation), based on the BT2 water vapour line list by Barber & Tennyson (2008), to determine the micro-turbulence velocity, the diffusion coefficient, and the advective mixing of molecules (including water vapour) as a function of depth. This new model grid of atmospheres and synthetic spectra has been computed for 100,000K > Teff > 400K, 5.5 > logg > 0.0, and [M/H]= +0.5 to -1.5, and the reference solar abundances of Asplund et al (2009). We found that the new solar abundances allow an improved (practically perfect) reproduction, for the first time, of the photometric and spectroscopic properties of M dwarfs, brown dwarfs, and extrasolar planets, and a smooth transition between the spectral type regimes.

14.00 Discussion

14.15 Water in evolved stars

Professor Jose Cernicharo, Centro de Astrobiología, Instituto Nacional de Técnica Aeroespacial, Spain

Water vapour is one of most abundant molecules in O-rich evolved stars and recently it has been found in a large variety of carbon-rich objects. While the formation of water in O-rich stars is well understood, the situation for C-rich objects is less obvious and warm photochemistry and shocks have been claimed as possible physical and chemical processes dealing with the formation of H$_2$O in AGB stars.

I will review the recent results from Herschel, the complexity of the interpretation of the data dealing with huge line opacities, and the different chemical processes invoked in the formation of water vapour. I will also analyze the potential of ALMA in observing maser lines of H$_2$O for which the Earth atmospheric transmission allow their observation from ground facilities paying particular attention to the 183.3 and 325 GHz maser lines of para water. Finally, I will discuss the water lasers that could be observed with PACS/Herschel arising from resonant levels in highly excited vibrational levels of H$_2$O.

14.45 Discussion

15.00 Tea

15.30 Water in exoplanets

Dr Giovanni Tinetti, University College London, UK

The science of extra-solar planets is one of the most rapidly changing areas of astrophysics. A combination of ground-based surveys and dedicated space missions has resulted in 540-plus planets being detected, and over 1200 that await confirmation – since 1995, the number of planets known has increased by two orders of magnitude. NASA's Kepler mission has opened up the possibility of discovering Earth-like planets in the habitable zone around some of the 100,000 stars it is surveying during its 3 to 4-year lifetime. The new Gaia mission is expected to discover thousands of new planets around stars within 200 parsecs of the Sun. Yet among the exoplanets detected or proposed, so far there is actually little resemblance to the morphology of the Solar System.

So now the key challenge is moving on from discovery, important though that remains, to characterisation: what are these planets actually like, and why are they as they are? A key factor driving the characterisation is the discovery of transiting planets, whose presence can be detected by the reduction in the brightness of the central star as the planet passes in front of it. Some 125 of the 530+ currently identified exoplanets are transiting planets. Most recently, we have been able to demonstrate that it is possible to use the wavelength dependence of the transit extinction to identify key chemical components in the planet's atmosphere. As a result, we have discovered for the first time molecules such as water vapour, methane and carbon dioxide in the atmosphere of an exoplanet from space or from the ground.

Finally, a new space mission is currently assessed by the European Space Agency: EChO, the Exoplanet Characterisation Observatory. EChO, will be the first dedicated mission to investigate the physics and chemistry of exoplanetary atmospheres. It will place our Solar System in context and will allow us to address fundamental questions such as: what are the conditions for planet formation and the emergence of life?

16.00 Discussion

16.15 Water in star and planet-forming regions

Professor Edwin A Bergin, University of Michigan, USA

In this talk Professor Bergin will discuss the astronomical search for water vapour in order to understand the disposition of water in all its phases throughout the process of star and planet formation. Gas-phase water is one of the dominant probes of this water cycle. Tracing the trail of water as it forms in space and is ultimately provided to forming terrestrial worlds is a key astrophysical goal Our ability to detect and study water vapour has recently received a tremendous boost with the successful launch and operations of the Herschel Space Observatory. Herschel spectroscopic detections of numerous transitions in a variety of astronomical objects, along with previous detections by other space-based observatories, will be threaded throughout this presentation. We will also stress the close link between astronomy, physics, and chemistry that represent the basis for the gains in our knowledge of the cycle of water. In particular, Professor Bergin will present observations of water vapour tracing the earliest stage of star birth where only a trace amount of water exists in the gaseous state. Instead water is found as an ice-coating on small tiny solid particles that are the seeds of Earth-like planets. When a star is born the local energy release by radiation liberates these ices in its surrounding envelope and powers energetic outflows that appear to be water-vapour factories. In these regions water vapour can be detected via tens of transitions over a broad energy range (10 K through over 1000 K) and this emission is an important tracer of the gas physical and chemical state.

Closer to the star a disk is formed from the collapsing gas cloud. Professor Bergin will end with a discussion of the distribution of water in the planet-forming disk where we are now detecting emission lines from both warm (T ~ 500 K) water vapour and cold (T ~ 50 K) water vapour throughout the entire extent of young analogs to our own solar system.

16.45 Discussion and closing remarks

17.30 End of meeting

Organiser, speaker and chair biographies

Dr France Allard, Centre de Recherche Astrophysique de Lyon, France (Speaker)
Dr France Allard is the first and a world renowned expert for nearly twenty years as an atmosphere modeller for very low mass stars (VLMs), brown dwarfs (BDs), and extrasolar giant planets (EGPs). She obtained a PhD in astrophysics at the Ruprecht Karls University in Heidelberg in 1990. She was recruited on a research grant at the University of Montreal for 3 years till 1993. After this appointment she occupied a position of sessional lecturer at the British Columbia University in astronomy for 2 years till May 1995, and became a research assistant at The Wichita State University for 2 years till 1997. Finally she was received as an invited professor at the Centre de Recherche Astrophysique de Lyon (CRAL) for 10 months till May 1998, and was received at a permanent responsibility CNRS position at CRAL till today. In June 2004, she obtained the Habilitation, and was among the most recent CNRS employee to be promoted at the level of Director of Research (CNRS) in 2008.

Among Dr Allard's achievements is the first realistic model atmosphere grid spanning the complete range of parameters of VLMs and BDs. This is soon to be followed in 2001 with one of the first study of dust clouds formation in VLMs and BDs atmospheres. These model atmosphere grids (NextGen '99, Cond/Dusty '01, BT-Settl '10) allowed several advances: i) for the first time the use of non-grey model atmospheres as a surface boundary conditions to interior and evolution models; ii) the determination of the temperature scale of VLMs; iii) the characterization of brown dwarfs at the stellar boundary via the lithium test and/or by spectral synthesis, and by realistic theoretical isochrones fitting; iv) the discovery and characterization of ever lower mass brown dwarfs (of surveys e.g. CFBDS, UKIDSS to name the most recent) the characterization of Hot Jupiters upon their discovery with the detection of water vapour in 2007; and vi) the constraint of the detectability of planetary mass objects and biosignatures using observing instruments (SPHERE, DARWIN among the most recent). Most recently, Dr Allard is also known worldwide for 2-3D radiation hydrodynamic simulations of the atmospheres of VLMs, BDs, and EGPs in presence of dust cloud formation and rotation since 2005.

Dr Stephen Ball, University of Leicester, UK (Chair)
Dr Stephen Ball is Senior Lecturer in Atmospheric Chemistry at the Department of Chemistry, University of Leicester, UK. His research interests lie in studying the reactive trace gases that drive chemical change in the lower atmosphere. The aim is to better understand how manmade and natural emissions interact with the chemistry of the troposphere to affect atmospheric composition, air quality and climate. To date, Ball's research has mainly focused on: the roles of nitrogen oxides in the polluted urban environment and in the chemistry of the atmosphere at night; the production of oxygenated volatile organic compounds from the atmospheric degradation of hydrocarbons; and biogenic emissions of iodine and its subsequent chemistry in the coastal marine atmosphere. In order to quantify such species at the high dilutions they occur in the atmosphere, he has developed ultra-sensitive instruments based on broadband variants of cavity ringdown spectroscopy which he regularly deploys in field work and for experiments at atmospheric simulation chambers. Cavity-based techniques are also applied in laboratory studies, for example, to measure absorption signals due to the water dimer at atmospherically important near-infrared wavelengths.

Dr Yuri Baranov, Institute of Experimental Meteorology, Russia (Speaker)
Dr Yuri Baranov was born in 1954 in Novgorod region of Russia. In 1980 he graduated from St Petersburg (former Leningrad) State University with specialization: “Theoretical and Applied Molecular Spectroscopy”. In 1982 he defended PhD thesis. Since 1980 Baranov has been with the Institute of Experimental Meteorology of the Russian Federal Agency on Hydrometeorology and Environment Protection. In 2001-2004, 2006-2007 and 2009 Baranov was invited to National Institute of Standards and Technology to carry out studies of collision induced absorption. His scientific interests include collision induced and continual absorption of IR radiation by the major atmospheric species, atmospheric spectroscopy.

Professor Edwin Bergin, University of Michigan, USA (Speaker)
Edwin Bergin is a leading scientist in the area of theoretical and observational studies of the chemistry and physics in star and planet forming molecular gas. He has also played an important role in a number of observational projects, including being a key member of the science team for NASAs Submillimeter Wave Astronomy Satellite (SWAS). Currently he is the principle investigator of a guaranteed time key program on the Herschel Space Observatory and serves as a co-investigator on several other key programs that place strong focus on the search for water in interstellar space. One of his specialties is the study of water vapour during the epoch of stellar birth and on the trail that leads to the formation of water-rich terrestrial worlds.

Professor Peter Bernath, University of York, UK (Organiser, Chair)
Peter Bernath received his BSc degree from the University of Waterloo (1976) and his PhD degree in physical chemistry from MIT in 1980. After a post-doctoral stint at the National Research Council of Canada, he became a faculty member at the University of Arizona from 1982-1990. In 1991 he took up a position as Professor of Chemistry and of Physics at the University of Waterloo, followed by a move in 2006 to the University of York in the UK. At York, he is Chair of Physical Chemistry and director of the York Centre for Laser Spectroscopy. His research interests are in the application of lasers and Fourier transform spectrometers to the study of molecular spectra. More recently, his interests have turned to molecular astronomy and atmospheric science. He is mission scientist for the Atmospheric Chemistry Experiment (ACE), on the SCISAT-1 satellite currently in low-earth orbit.

Professor Jose Cernicharo, Centro de Astrobiología, Instituto Nacional de Técnica Aeroespacial, Spain (Speaker)
Not available at time of printing

Dr Tom Gardiner, National Physical Laboratory, UK (Speaker)
Tom Gardiner has 20 years of experience on the development and implementation of advanced trace gas monitoring techniques, and the assessment of the calibration requirements and uncertainty analysis of such measurement techniques. This work has included the development of new laser-based techniques for remote sensing systems, including a novel injection-seeded optical parametric oscillator and a near-infrared tunable diode laser spectrometer. His extensive field measurement experience has included more than a dozen international campaigns studying tropospheric and stratospheric science issues. These campaigns have included ground-based measurements involving Fourier Transform and laser heterodyne spectrometers, remote measurements using UV and IR differential absorption lidars, and balloon-and aircraft-based measurements with laser absorption spectrometers. He is a member of the Infrared Working Group of the international Network for the Detection of Stratospheric Change, and sits on the steering committee of the GCOS Reference Upper Air Network.

Dr Paul Green, Imperial College London, UK (Speaker)
Dr Paul Green studied at Manchester University (MPhys 1998) and Imperial College (PhD 2003) after which he has been working at Imperial College as a Postdoctoral Researcher. He became a Scholar Freeman of London via the award of a post-graduate scholarship from the Worshipful Company of Scientific Instrument Makers in 2001 and elected as a member of the Institute of Physics, and Fellow of the Royal Meteorological Society in 2005.

Dr Green's research interests centre on tropospheric clear-sky and cloud radiative effects in the far-IR (16-125μm). His PhD thesis work concentrated on clear-sky spectroscopy, in the form of the water vapour pure rotation band continuum. I have also undertaken studies of the radiative effects of cirrus cloud in the infrared, with flight campaigns both in the UK and Australia looking at both frontal and tropical convection-generated cirrus, as well as the arctic ground-based RHUBC measurement campaign.

Dr Green is the current TAFTS instrument mentor and has been involved with the development, maintenance and deployment of this instrument on various experimental campaigns.

He is currently back studying the far-IR water vapour continuum through analysis of measurements from the RHUBC and CAVIAR projects.

Professor Jean-Michel Hartmann, Université Paris, France (Speaker)
Jean-Michel Hartmann attended the Ecole Centrale Paris where he got an engineer degree (1983) and a PhD (1986) before being hired by the French national center for scientific research (CNRS). After ten years (1983-1992) in the LEM2C in Ecole Centrale, he joined the Orsay university campus (LPMA and LPPM labs), before joining the LISA in Créteil in 2000. He is now Directeur de Recherche for the CNRS. His research, mainly theoretical, is in the area of spectroscopy and of its applications for atmospheric soundings, with emphasis on the effects of collisions (of pressure) on the shape of absorption/emission spectra of molecular gases, a subject on which he has co-written a recently published book.

Dr Joseph Hodges, National Institute of Standards and Technology, USA (Speaker)
Joseph T Hodges has degrees in Mechanical Engineering from Purdue University (BSc 1981) and the University of Wisconsin-Madison (PhD 1989). He was a postdoctoral fellow for two years at l'Institut Français du Pétrole, and since 1991 he has been a research scientist at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland USA. His research interests include laser combustion diagnostics, light scattering and absorption properties of aerosols, development of advanced primary standards for the generation and measurement of humidity, and high-resolution cavity-enhanced laser absorption techniques for high-accuracy measurements of spectroscopic line parameters and gas concentration.

Dr Rod Jones, University of Cambridge, UK (Speaker)
Roderic L Jones is Professor of Atmospheric Science at the Department of Chemistry, University of Cambridge. He obtained his first degree in Physics at the University of Oxford before obtaining a DPhil in Atmospheric Physics, also at Oxford and spent 5 years at the UK Meteorological Office before moving to the Department of Chemistry in Cambridge in 1990. His main research interests are in studies of the structure and composition of the atmosphere, focusing on a wide range of issues from local air quality to global climate change, with an emphasis on both the detection of trends, and studies of the processes which control the chemical composition and physical structure of the earth's atmosphere.

A particular interest of his research team is the development and exploitation of novel observational techniques, ranging from ultra-sensitive spectroscopic techniques which form the basis of his laboratory studies of water vapour absorption, through to miniaturised chemical sensors and sensor network systems. He has over 100 peer reviewed publications, has been closely involved with numerous national and international scientific assessments and currently holds NERC, EPSRC and EU research awards totalling approximately £5M.

Professor Claude Leforestier, Université Montpellier, France (Speaker)
Claude Leforestier obtained his BSc (1973) and PhD (1980) degrees from the Université Paris Sud in Orsay and was a postdoctoral fellow at the University of Texas in Austin (1980-1981). He was visiting professor at the University of California in Berkeley (1992-1993). After holding a research associate position (1975-1987) at the French national research centre, he became Theoretical Chemistry Professor at the Université Paris Sud in Orsay. In 1995 he moved to the Université Montpellier. He co-authored more than 100 scientific publications. His field of interests concerns Molecular Reaction Dynamics, with special emphasis on Molecular Spectroscopy. Mainly interested in methodological developments, he pioneered *ab initio* molecular dynamics (1978), and investigated the atmospheric UV photodissociation of ozone. Recent work concerns methodological developments for the calculation of highly excited states of polyatomics and of molecular clusters.

Dr Pavlo Maksyutenko, Paul Scherrer Institute, Switzerland (Speaker)
Pavlo Maksyutenko (1979) graduated Kyiv Polytechnic Institute, Ukraine, with a MSc degree in Applied Physics in 2003. Next year he joined the group of Professor Thomas Rizzo at École Polytechnique Fédérale de Lausanne where he got his PhD in 2008, studying multiple-resonance vibrational spectroscopy of water and methanol molecules. He spent 1.5 years as a PostDoc in the laboratory of Professor Ralf I Kaiser at the University of Hawaii studying reaction dynamics in crossed molecular beams, relevant to planetary atmospheres, combustion and interstellar medium. Recently he moved back to Switzerland to work as a PostDoc in Nonlinear Optics laboratory of General Energy department at Paul Scherrer Institute.

Dr Eli Mlawer, Atmospheric and Environmental Research, Inc, USA (Speaker)
Dr Mlawer is a Senior Scientist and the Leader of the Atmospheric Composition and Radiation Section at AER. His main research interests are atmospheric radiative transfer and climate. Dr Mlawer has primary responsibility for the design, implementation, and validation of RRTM, a radiative transfer model for climate applications used by many climate and weather prediction models. He is the co-leader of the Continual Intercomparison of Radiation Codes (CIRC) effort to evaluate the quality of radiation codes used in climate simulations. Dr Mlawer was co-Principal Investigator of the two Radiative Heating in Underexplored Bands Campaigns (RHUBC), field experiments that took place in northern Alaska (2007) and Chile (2009) directed at increasing our understanding of key radiative processes in the far-infrared spectral region. He is the developer of the MT_CKD water vapour continuum model, a key component in the majority of existing atmospheric radiative transfer models. Dr Mlawer received a BA degree in mathematics and astronomy from Williams College, a BA and MA in physics from Cambridge University, and a PhD in physics from Brandeis University.

Dr Stuart Newman, Met Office, UK (Speaker)
Stuart Newman obtained a BSc in Chemical Physics at the University of Bristol in 1996, and stayed in Bristol to complete a PhD on the electronic spectroscopy of atmospherically-important molecules using cavity ring-down and Fourier transform spectroscopy. Since joining the Met Office in 1999 Stuart has used airborne interferometer observations to investigate issues of importance to infrared remote sensing, including sea- and land-surface emissivity, fundamental spectroscopy, satellite calibration and validation, and 1-dimensional variational retrievals of atmospheric species. Most recently Stuart has worked on the remote sensing of

volcanic ash following the Eyjafjallajökull eruption, alongside water vapour continuum studies as part of the CAVIAR consortium.

Dr Oleg Polyansky, Russian Academy of Sciences, Russia (Speaker)
Oleg Polyansky received his diploma degree in radiophysics from the Gorky State University, USSR, (1979). The same year he became a junior research fellow at the Applied Physics Institute of the Russian Academy of Science (USSR at that time). His PhD work has been done at this Institute and defended at Tomsk University in 1993. By that time he was a senior research fellow of the same institute. After receiving his PhD he won the Humboldt fellowship, which he spent with Professor Manfred Winnewisser and Professor Per Jensen in Giessen, Germany. In 1995 he took a postdoc position at University College London with Professor Jonathan Tennyson. He spent the years 2004 to 2006 as a researcher at Ulm University, Germany and the years up to 2008 as a visiting professor at University College London. At the moment he is a group leader and leading research fellow in his home town (now called Nizhny Novgorod) at the Applied Physics Institute, Russia.

His research interests are in the development and application of methods for the high precision calculation of the spectra of small molecules and ions, and analysis of their spectra at high excitation, including high temperatures and dissociation.

Dr Igor Ptashnik, University of Reading, UK (Speaker)
Igor V Ptashnik graduated from the Physics Department at the Novosibirsk State University (Russia) in 1984 (master degree in Optics and Spectroscopy). He worked for 6 years as an experimentalist in the Institute of Atmospheric Optics, Tomsk (Russia). In 1990 he changed his area of interest from experimental study to numerical simulation of atmospheric absorptional processes. In 1996 he received PhD degree from Russian Academy of Science (RAS) for thesis "Mathematical modelling of the optical absorptional remote sensing of atmospheric gases". In 2001-2003 Dr Ptashnik worked in the Department of Meteorology, University of Reading investigating different mechanisms of the absorption of solar radiation by water vapour in the Earth atmosphere. In 2007 he defended a 'Doctor of Science' degree of RAS with the thesis "Continuum absorption by water vapour within near-infrared bands".

Currently DrSc Ptashnik is a senior staff scientist in the Institute of Atmospheric Optics RAS (Russia). Since 2007 he has also been working in the University of Reading as a Senior Research Fellow and coordinator of CAVIAR consortium (Continuum Absorption at Visible and Infrared and its Atmospheric Relevance).

Professor Keith Shine FRS, University of Ready, UK (Organiser)
Keith Shine is Professor of Physical Meteorology at the University of Reading, UK. He has worked for around 30 years in climate science, specifically on aspects of radiative transfer as they relate to climate and climate change and has, for example, served as a lead author on the assessment reports of the Intergovernmental Panel on Climate Change. He was elected as a Fellow of the Royal Society in 2009. He is the Principal Investigator of the UK-funded consortium called CAVIAR (Continuum Absorption of Visible and Infrared Radiation and its Atmospheric Relevance) and has had a long involvement in understanding the radiative role of water vapour in the Earth's atmosphere.

Dr Jonathan Taylor, Met Office, UK (Organiser, Chair)
Jonathan graduated from the University of Reading with a Joint Honours Degree in Physics and Meteorology in 1988. He then joined the Meteorological Research Flight at the UK Met Office and whilst working for the Met Office completed a PhD, in 1993, at University of Reading on The Remote Retrieval of Stratiform Water Cloud Radiative and Microphysical Properties - using data gathered by the Met Office C130 aircraft.

Jonathan has been involved in airborne research observations throughout his career and his team utilise the FAAM Bae146 Atmospheric Research Aircraft. Jonathan is now Head of Observations Based Research at the Met Office managing all the Met Office involvement in airborne research observations and overseeing the boundary layer measurement site at Cardington Bedfordshire.

One focus of Jonathan's research has been the development of new techniques to better utilise data from the Infra-red Atmospheric Sounding Interferometer (IASI) which flies on the Metop satellite and is co-chairman of the Eumetsat hosted IASI Sounding Science Working Group. Jonathan has served as an associate editor for the Quarterly Journal of the Royal Meteorological Society. He won the LF Richardson Prize from the Royal Met Soc in 1996 and the LG Groves Memorial Prize for Observations in 2009.

Professor Jonathan Tennyson FRS, University College London, UK (Organiser)
Jonathan Tennyson gained a BA in Natural Sciences from King's College, Cambridge in 1977 and a PhD in Theoretical Chemistry from the University of Sussex in 1980. He spent a productive two years as Royal Society Western European Exchange Fellow at the University of Nijmegen in the Netherlands, In 1982 Tennyson joined the Theory Group at Daresbury Laboratory. He was appointed a "New Blood" lecturer at University College London in Theoretical Atomic Physics in 1985. He became Professor of Physics in 1994; took over as Head of Department in 2004 and as Massey Professor of Physics in 2005. He was elected an FRS in 2009. His research interests cover a range of topics on the theory of small molecules. In particular he computes spectra of these molecules (such as water) and collide electrons (and occasionally positrons) with them. He is interested in the astrophysical, atmospheric and other consequences of these processes. He recently started a new project, ExoMol, aimed at calculating comprehensive line lists for models exoplanets and other hot atmospheres.

Dr Giovanni Tinetti, University College London, UK (Speaker)
Dr Giovanna Tinetti is a reader at University College London and a Royal Society University Research Fellow. She has coordinated at University College London a team on exoplanets since 2007 and was recently appointed editor of ICARUS for the exoplanet section. Tinetti has been working on exoplanet characterisation since 2001 when she joined the NASA Astrobiology Institute team at the Jet Propulsion Lab in Pasadena. With colleagues Tennyson and Barber at University College London, she pioneered the detection of water vapour in an exoplanet atmosphere using transmission band photometry in the IR with the Spitzer Space Telescope (Tinetti et al, Nature, 2007), a result confirmed a few months later by spectroscopic observations with Hubble in the Near-IR (Swain, Vasisht, Tinetti, Nature, 2008). The same Hubble data showed the additional presence of methane in the same atmosphere, a discovery awarded with the JPL-Edward Stone Award and NASA Group Achievement Award, in 2009. Tinetti is currently the lead scientist of the ESA mission concept EChO (Exoplanet Characterisation Observatory), the first space mission devoted to the observation of exoplanet atmospheres.

Dr Andrei Vigasin, Russian Academy of Sciences, Russia (Chair)
Andrei A Vigasin, graduated from Physics Department, Lomonosov Moscow State University, in 1972. He is currently a Leading Research Scientist in the Obukhov Institute of Atmospheric Physics, Russian Academy of Sciences in Moscow. He earned his PhD (1978) and DoctSci (1995) degrees from Moscow State University, Physical and Chemical Departments, respectively. His main scientific interests are presently in the domain of spectroscopy, statistical physics, and quantum chemistry of weakly interacting molecules, which may have an impact on radiative and physico-chemical processes in the atmosphere. He is particularly concerned with collision-induced and water vapour continuum absorption phenomena. In 1998 and 2003 he co-edited (with Z Slanina and C Camy-Peyret, respectively) multi-author books entitled "Molecular Complexes in Earth's,

Planetary, Cometary, and Interstellar Atmospheres'', The World Scientific, and "Weakly Interacting Molecular Pairs: Unconventional Absorbers of Radiation in the Atmosphere", Kluwer Academic Press.

Professor Ewine van Dishoeck, Leiden Observatory, The Netherlands (Organiser)
Ewine F van Dishoeck is a full professor of astronomy at Leiden University, the Netherlands, where she received her PhD in 1984 cum laude. From 1984-1990, she held positions at Harvard, Princeton and Caltech before moving back to Leiden in 1990. As of 2008, she is also an external scientific member of the Max Planck Institut für Extraterrestrische Physik in Garching, Germany. Her research group focusses on molecules in star- and planet-forming regions and the importance of molecules as diagnostics of the physical processes, using observations at submillimeter and infrared wavelengths. She holds many national and international science policy functions, including scientific director of the Netherlands Research School for Astronomy (NOVA), member of the Board of the Atacama Large Millimeter/submillimeter Array (ALMA) and PI of the Herschel key program on 'Water In Star-forming regions with Herschel'(WISH). She has received various honors and awards for her research.

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