Switch on the weather forecast any evening and one is left in no doubt as to the importance of water in the Earth’s atmosphere: will the water be gaseous (humidity), liquid (clouds, rain), solid (snow, ice or hail) or taken up by aerosol (haze) particles? The long-term role of water in our climate, and of course any change in our climate, is no less profound. The water vapour is both the dominant absorber of incoming sunlight and the major greenhouse gas, so any climate model has to adequately account for its behaviour.

While many aspects of how the water molecule absorbs and emits light in our atmosphere are becoming increasingly well understood, some remain scientifically challenging. For example, a thorough understanding of the actual shape of individual water absorption lines is crucial for correctly modelling absorption by water vapour. This is necessary not only for climatic reasons but also because many remote sensing experiments, both space and ground based, require a detailed understanding of this absorption so that the characteristic signatures of other, trace species can be recovered. As discussed by Ngo et al. [1], there is now incontrovertible evidence that the true line shape, at line centre and in the near wings, departs significantly from the Voigt profile that has traditionally been used to represent the change in water line profiles as a function of temperature and pressure. However, what one should use instead of Voigt profiles remains a matter for debate, which is informed by high-precision experiments such as those reported by Hodges et al. [2].

The radiative impact of atmospheric water vapour (and its role in remote sensing) depends not only on the tens of thousands of individual absorption lines but also on the so-called water vapour continuum, which varies relatively smoothly with wavelength from visible to microwave wavelengths. The continuum has been most intensively studied in the mid-infrared ‘window’ (wavelengths from approx. 8 to 12 μm) but, outside of this region, its strength and temperature dependence, particularly in atmospheric conditions, are less well characterized. In addition, there has been a long-lasting and robust debate as to the underlying cause of the continuum, it probably being due to some combination of the far wings of individual spectral lines of the water monomer and absorption owing to water dimers and other bimolecular complexes (e.g. H₂O–N₂). Many radiative transfer codes used in weather prediction and climate models use the semi-empirical representation of the water vapour continuum from the CKD (Clough–Kneizys–Davies) and MT_CKD (Mlawer–Tobin–Clough–Kneizys–Davies) family of models; Mlawer et al. [3] provide a detailed description of the newest version of this model and describe how
recent laboratory and atmospheric observations have led to significant revisions when compared with earlier versions. Such models are still not sufficiently constrained by observations in important parts of the spectrum. New laboratory measurements of the continuum owing to water–air mixtures in the near-infrared windows by Ptashnik et al. [4] indicate that absorption is up to about 100 times stronger than given by the semi-empirical models. Baranov & Lafferty [5] present new observations of the continuum at 4 and 10 \( \mu \)m; while the differences with the semi-empirical models are greatest at the shorter wavelengths, the work stresses that, even in the better characterized mid-infrared region, the semi-empirical models still do not fully reproduce the observed spectral and temperature dependence.

Direct atmospheric measurements of continuum absorption are more relevant to the problem of understanding the atmospheric impact of the continuum, but generally more difficult than laboratory measurements, because of challenges in properly characterizing the atmospheric state, and in calibrating field spectrometers. Gardiner et al. [6] demonstrate the necessary steps required for radiative calibration of a sun-pointing spectrometer, and show that the spectral irradiance reaching the surface can be measured to better than 6 per cent uncertainty. Airborne and satellite measurements analysed by Newman et al. [7] indicate broad agreement with the laboratory measurements in Ptashnik et al. [4], but they present evidence that there may be a hitherto undetected temperature dependence in the continuum of water–air mixtures at atmospheric temperatures. The far-infrared airborne measurements by Green et al. [8] are the first to cover the whole of the water monomer rotation band using a single instrument. Their analyses indicate agreement with existing continuum models, within known uncertainties, at wavelengths below about 30 \( \mu \)m, but, at longer wavelengths, their measured continuum is up to 50 per cent stronger.

Significant advances in the \textit{ab initio} quantum mechanical modelling of the absorption by water dimers have been made in recent years, but still a full theoretical solution is computationally so demanding (it is formally a 12-dimensional problem) that effective simplifications have to be sought. Tennyson et al. [9] examine and compare methods for removing some simplifications in earlier approaches, particularly the simultaneous treatment of the inter- and intra-molecular oscillations of the dimer. Leforestier [10] achieved good agreement between observations and his calculations, when the monomers were treated as being rigid but with the rotational constants of the monomer depending on the dimer geometry. Baranov et al. [11] consider H\(_2\)O–N\(_2\) collision-induced absorption at wavelengths near 4 \( \mu \)m, and find good agreement between laboratory measurements and \textit{ab initio} theory.

Laboratory work on the water monomer has continued to probe the behaviour of the water molecule. In particular, the group from École Polytechnique Fédérale de Lausanne has pioneered the use of multi-photon spectroscopy to probe the ladder of vibrational states leading all the way to dissociation, moving way beyond the scope of conventional spectroscopic studies. This work has also led to a greatly improved dissociation energy for water and the first observation of quasi-bound states of the molecule above dissociation. The latest experimental progress in this area is discussed by Matsyutenko et al. [12]. Such measurements of course provide a challenge for theory, in particular because water has become a benchmark system for full \textit{ab initio} quantum mechanical
treatments. Polyansky et al. [13] discuss how theory is rising to these challenges and present encouraging results on how their calculations reproduce the latest dipole measurements. Calculated transition dipoles and the associated transition intensities and Einstein-A coefficients are playing an increasingly important role in practical applications of spectroscopy such as those found in astrophysics.

An important application of calculated water spectra is the identification of water in the atmospheres of extrasolar planets, given that, so far, such observations have only been made on ‘hot Jupiters’ whose modelling requires understanding of the absorption and emission spectra of key molecules such as water at temperatures too elevated for standard laboratory line lists. Tinetti et al. [14] discuss the modelling and data requirements necessary to interpret the presently available observations and the urgent need for improved observational data to resolve issues surrounding the interpretation of the exoplanetary spectra obtained thus far. Their results demonstrate the importance of pressure-broadening of water lines in models of exoplanet atmospheres, particularly at long wavelengths.

The spectra of brown dwarfs and cool stars differ from those of transiting exoplanets in that the light source is internal; however, they have similarities that constructing reliable models and interpreting their spectra requires for extensive datasets of molecular transitions with a particular emphasis on water. The changes in these models occasioned by the use of the most recent spectroscopic dataset for hot water are the theme of the paper by Allard et al. [15]. Water is also crucial at the lower temperatures involved in star formation: star-forming regions are being increasingly monitored by spaceborne missions such as the Herschel satellite. Bergen & van Dishoeck [16] illustrate how monitoring water spectra give insight into the collapse and cooling necessary to form stars.

The ‘Water in the gas phase’ Discussion Meeting took place at the delightfully appointed Kavli Centre, Chicheley Hall, Chicheley, UK, on 13 and 14 June 2011. We were fortunate that meteorologically the water did indeed remain in the gas phase, allowing discussions and poster sessions to be held outside and the principles of classical mechanics to be tested on the croquet lawn.

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