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A Comparison of Water Vapour Line Lists

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Abstract.
M dwarf spectra, at wavelengths beyond 1.35 μm, are dominated by water vapour yet terrestrial water vapour makes it notoriously difficult to make accurate measurement from ground-based observations. We have used the short wavelength spectrometer on the Infrared Space Observatory to obtain the 2.5–3.0 μm region. The observations show a good match with synthetic spectra based on the Partridge & Schwenke (1997) line list though not with the SCAN (Jorgensen et al. 2001) line list. Nonetheless, the Partridge & Schwenke calculations for water vapour lines still need to be extended to higher energy levels with good convergence for reliable modelling of hot water vapour. Then water bands can assume their natural role as the primary tool for the spectroscopic analysis of M stars.

1. Introduction

More than two-thirds of stars within 10 parsecs are M dwarfs and it is very probable that this number density prevails throughout our Galaxy. Unless there is a sharp turn-down in the stellar mass function, they and even lower mass objects are a major component of the Galaxy's mass. The dominant source of opacity for the late-type M dwarfs and brown dwarfs is water vapour which easily forms in their relatively high pressure, low temperature atmospheres. Leaps in theoretical molecular quantum mechanics and computer hardware capabilities mean that it is possible to perform ab initio calculations to accurately predict the frequency and intensity for ro-vibrational transitions for water vapour. This means that it is no longer necessary to extrapolate laboratory measurements for water vapour to the temperature and pressure regimes found in the atmospheres of M dwarfs.

The preponderance of water vapour in the Earth's atmosphere makes it very difficult to observe its spectral signature in stars. At near-infrared wavelengths, where cool stars emit most of their flux, the strongest water vapour absorption band is centred around 2.65 microns where the atmosphere is opaque. The advent of the Infrared Space Observatory has for the first time allowed observations

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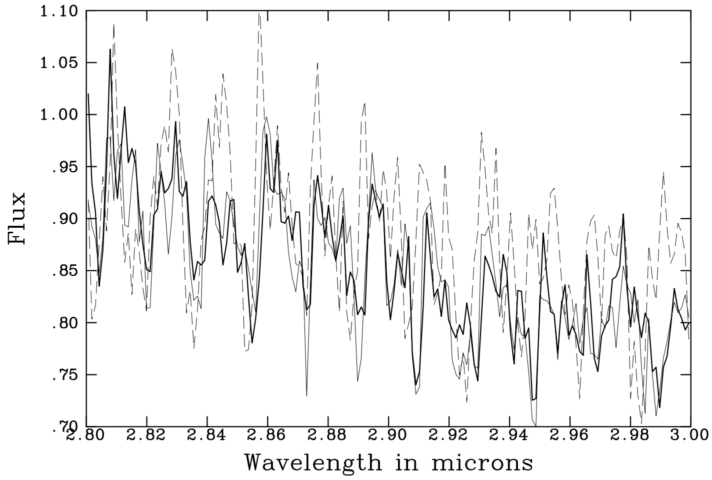

Figure 1. GJ 406 compared with 3000 K synthetic spectra using the MT and PS line lists. The observed spectra and PS model are shown as solid thick and thin lines respectively and the MT model as a dotted line. The match of water bands between observations and model is considerably better for the PS model.

to be made at the peak of water vapour absorption in cool stars. Such data are impossible to obtain from terrestrial sites.

2. Available Water Line Lists

The crucial opacity for M stars across the range of our observed spectra is water vapour. A useful model atmosphere thus needs to include an appropriate water line list. There are several different sources of water data and a few of them have been investigated here. A reliable water line list needs: 1. a good (electronic) potential energy surface; 2. well converged nuclear motions (i.e vibration-rotation) calculations; 3. a reliable dipole surface. To date, it is not yet possible to a get a completely reliable *ab initio* potential surface, so all the line lists discussed in this paper used surfaces which have been adjusted to reproduce laboratory spectroscopic data for water. Fitting to lab data can cause problems in regimes where such data are unavailable (Polyansky et al. 1997a). Conversely tests (Lynas-Gray, Miller & Tennyson 1995) have shown that *ab initio* dipole surfaces are much more reliable than the ones fitted to experimental data.

The water vapour data investigated in this paper are from Miller et al. (1995, known as the MT list), from Partridge & Schwenke (1997, known as the PS or AMES list), from Jorgensen et al. 2001 (known as SCAN), and from Viti (1997, known as the VT2 line list) which superseded the MT and VTP1 line lists (Viti, Tennyson & Polyansky 1997). MT is a relatively small list (10 million lines) which used, by today's standards, a rather inaccurate potential. VTP1 energy surface is much more accurate than MT but it is still not complete

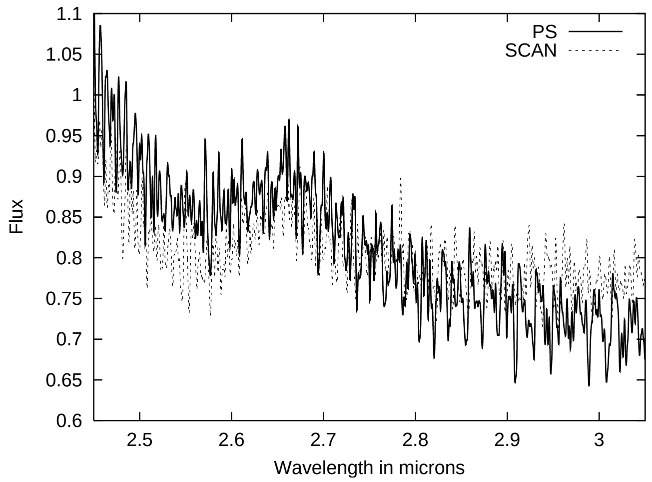

Figure 2. Comparison between synthetic spectra at 3100 K using the SCAN and PS line lists.

enough for stellar models. VT2 is a much larger line list ($>$ 300 million lines) which uses a potential surface reliable for higher vibrational states. However, due to serious computer format corruption problems this list could not be included in model atmospheres calculations.

3. Spectral Analysis

For this analysis we computed spectral energy distributions for a range of model atmosphere parameters: effective temperatures, $T_{\rm eff} = 2700$ — 3900 K, metallicities [Fe/H] $= +\,0.5$ — -1.5 and gravities $\log g = 0.0$ — 5.5. These were generated using the temperature structures from the model atmospheres of Hauschildt, Allard & Baron (1999) by the WITA6 program (Pavlenko 2000). We also used synthetic spectra from the PHOENIX model atmosphere code (NG5 - Hauschildt et al. 1999).

To provide an idea of the improvement since our previous work (Jones et al. 1995), in Fig. 1 we compare GJ 406 with 3000 K synthetic spectra generated using the PS and MT lists. As with Jones et al. (1995) we found that the intensities of the water band strengths seem to be reasonably well determined. However, we find that the PS line list prediction of bands with wavelength is a substantial improvement on the previously used MT line list. We also investigated using the SCAN line list (Jorgensen et al. 2001) and in Fig. 2 compare this to the PS list. As with our previous comparisons to the SCAN list (Jones et al. 1996) we find the predicted shape of the water bands as well as the structure of the bands are rather different from other models and observations. As expected from the scale of the calculation and previous comparisons with observations (e.g., Allard et al. 2000) we find that the PS line list is the most useful water line list available for our observed data. An illustration of the quality of the fit can be seen in Fig. 4. In Jones et al. (2001) we discuss why

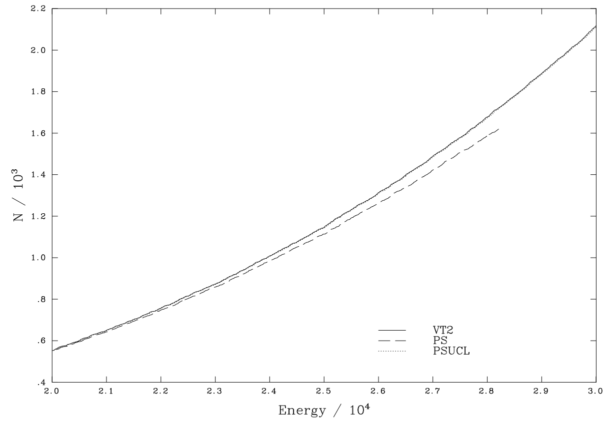

Figure 3. Number of energy levels as a function of energy for PS (dotted) and VT2 (continuous) line list for J = 17. The PS line list stops at 28000 cm^{-1}.

our best fit temperature for GJ406 is relatively high in comparison to literature values obtained with a variety of different methods.

3.1. Completeness of the PS line list?

For model atmospheres with effective temperatures in the range 2000 — 4000 K, Boltzmann considerations suggest that transitions involving states with J = 20 — 30 are the dominant sources of opacity. We find two problems with the PS line list: (i) first of all, it does not reach 30000 cm^{-1} for any J apart from $J = 0$. On average it gets to 28000 cm^{-1}. (ii) Secondly, even by truncating energy levels to 28000 cm^{-1}, VT2 still has more levels than PS has for high J, for example, at $J = 17$, VT2 gives 100 energy levels more than PS below 28000 cm^{-1}. From the number of energy levels missing for each J we estimate that PS omits $\sim$ 30 % transitions up to $J = 10$; $\sim$ 50% up to $J = 20$; and $\sim$ 60% up to $J = 28$.

As a test, a new set of energy levels using the PS potential energy surface, the same atomic masses as PS and VT2 nuclear motion parameters, were computed. This new set of energy levels is known as PSUCL (see Polyansky et al. 1997b for further comparisons). This was done to test the variational convergence for the same potential energy surface. An example of the energy levels comparison with VT2 and the new calculations is shown for $J = 17$ in Fig. 3. The calculations performed with the PS potential energy surface are in close agreement with VT2 which suggests that the lack of states in the PS line list is due to poor convergence and not to differences in the potential energy surface used. In fact, close examination of the parameters of the PS calculation strongly suggests that their decision not to increase the size of the Hamiltonian matrix beyond that used for $J = 4$ resulted in poorly converged calculations for higher states with high J. This decision undoubtedly saved them from some of the computational problems experienced in the computation of the VT2 line list (Viti 1997).

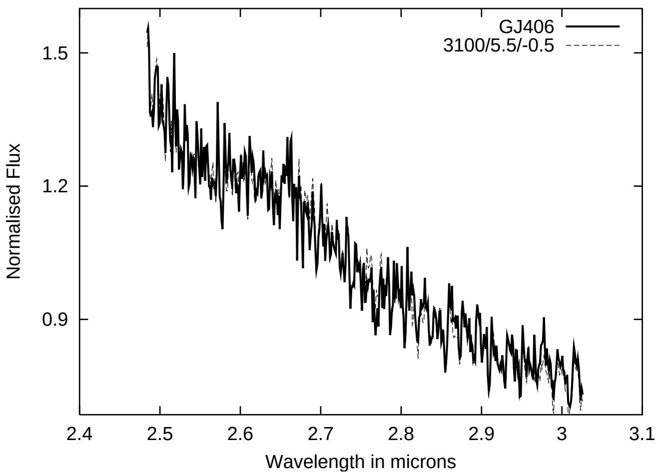

Figure 4. The observed spectrum of GJ 406 compared to a 3100 K, log g = 5.5, [Fe/H]=–0.5 synthetic spectrum.

For low-J energy levels, PS's calculations give superb results, reproducing experiment with a much higher accuracy than than VTP1 or VT2. However, for higher rotational states, particularly those with $J > 20$, we find that a very high proportion of rotational states which ones expects to be degenerate in fact show significant splittings in the PS line list. This splitting is not shown in VTP1, VT2 or in PSUCL. In particular for the levels with high K_a and with K_c odd (where K_a and K_c are the projections of J on the A and C principal axes of rotation of asymmetric top molecules), all lie below the ones with K_c even for levels with which they should be quasi-degenerate. Since the PS calculation truncates variational rotation-vibration calculations with 7500 energy-selected basis functions independent of the rotational parity this means that the K_c odd calculations will contain states of higher cut-off energy than the K_c even calculation. The variational principle means that the K_c odd states will be better converged and hence lower in energy.

This causes two problems. Firstly, artificial splitting of lines means that it is difficult to use the list for line assignments (Polyansky et al. 1997a). The second is more subtle. An important consideration in radiative transport is how the line absorptions fill in gaps in the spectrum. Two transitions which, to within their linewidth, are coincident will have less effect on the opacity than two separate transitions. Artificially doubling the number of lines for these J values is likely to cause the strength of water vapour bands at low resolution to be overestimated.

4. Conclusions

Observations of water vapour indicate that the PS line list predicts the positions and intensities of water vapour well enough to use for the determination of effective temperatures. The PS line list is a substantial improvement on the

MT line list which has been widely used for the generation of synthetic spectra of M dwarfs. The SCAN line list produced results substantially different from the observations and other models. The effective temperatures we determined are reasonably consistent with other methods of temperature measurement. Although the complex spectral energy distributions of cool dwarfs caused by water vapour have traditionally hampered reliable temperature determinations, it now seems feasible that observations of water rich regions coupled with the next generation of water vapour line lists might become the method of choice for the temperature determination of cool dwarfs.

However, a further conclusion of this work, in agreement with that of Allard et al. (2000), is that the presently available water line lists are still not good enough to generate accurate spectroscopic models of cool stars. These line lists have however been instrumental in improving the interpretation of hot water, e.g. in sunspots (Polyansky et al. 1997b); as a result there are now significantly more experimental data available on water (Tennyson et al. 2001). These data are being used to greatly improve the effective potential energy surfaces for water which, when combined with the improved dipole surface due to Schwenke & Partridge (2000), should make an excellent starting point for generating a new line list. Experience, such as the tests performed in this paper, show that all aspects of such calculations need to be of very high quality if a satisfactory water opacity is to be obtained.

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