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Hot Water in Cool Stars: the computation of the water linelist

S. Viti, J. Tennyson, O. L. Polyansky, S. Miller

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

1. Introduction

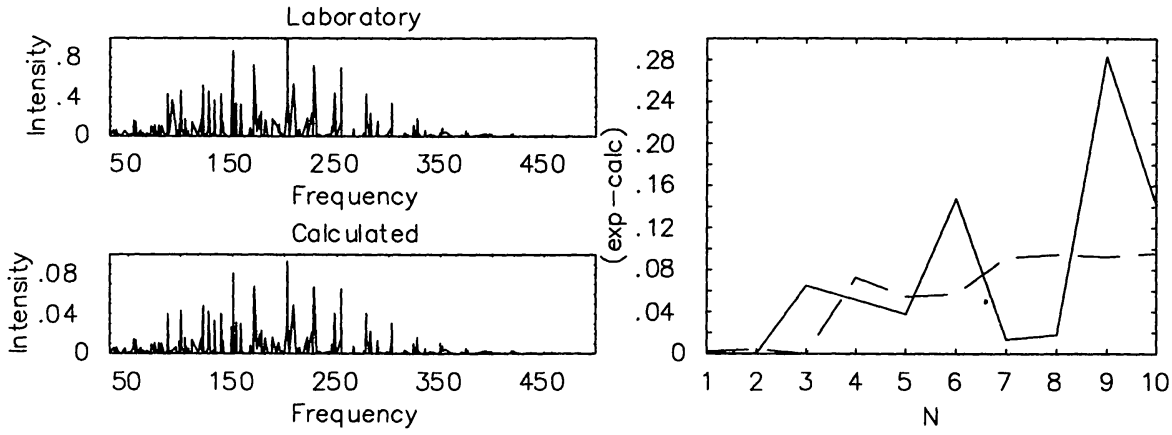
Comparisons of synthetic and observed spectra of cool stars show that a complete ab initio calculation of the hot water vapour transitions is urgently needed. At high temperatures ($\geq$ 1000K), spectroscopic calculations of the water spectrum are highly inaccurate, unless a full quantum mechanical approach is used. Such an approach was pioneered by Tennyson & Sutcliffe (1982). New codes use wavefunctions calculated explicitly on a grid of points (Discrete Variable Representation, DVR) rather than using basis sets (Finite Basis Representation, FBR). The latest 3-D program using a DVR method is called DVR3D (Tennyson, Henderson & Fulton, 1994). The computation for the water linelist has to include all levels up to 30000cm^{-1} above the ground state for J up to 40 in order to be applicable for model atmospheres of cool stars. The aim is to give an accurate representation for transitions longward of 0.2μm with accuracy better than 0.1cm^{-1}.

2. A Reduced Water Linelist

Using the program suite DVR3D we computed a preliminary water linelist which includes all the angular momentum states up to $J = 38$ for the ground vibrational state. The energies and the wavefunctions were generated using an electronic potential energy surface, PJT1, computed by Polyansky, Jensen & Tennyson (1994). The dipole transitions were computed using the dipole surface of Wattson & Rothman (1992). The intensities of the water lines at each wavelength were then calculated at $T = 300$K and compared with the very accurate laboratory measurements by Kauppinen, Karkkainen & Kyro (1979). The comparison shows the accuracy of this preliminary water linelist (see left hand side figure). We compared our calculations with values measured by Bernath et al. (private communications) at $T = 1823$K and found very good agreement. We also assigned all the relevant quantum numbers for many lines.

3. The Full Water Linelist: First Results

For this more complete calculation we used the electronic potential surface PJT2 by Polyansky, Jensen & Tennyson (in preparation) which is the most reliable for higher vibrational states. From the energy levels calculated so far, the accuracy has improved: the right-hand side figure shows the difference in energy levels



between the preliminary results and HITRAN (Rothman et al. 1987) and the new results and HITRAN (dashed line). Each N represents a group of energies which differ by the same amount from HITRAN energy levels: the new values never differ from the HITRAN values by more than 0.1cm^{-1}.

4. Conclusions

Miller et al. (1994) produced a water linelist which reached up to 11000cm^{-1}. This list has been incorporated in the model atmosphere code PHOENIX (see for example Allard & Hauschildt 1995) to compute synthetic spectra of M dwarfs. Comparisons of the produced synthetic spectra with high quality observations show that the total opacity is underestimated, overall at short wavelengths; we hope that with the inclusion of the new linelist this problem will be solved. The linelist will be also used to reproduce spectra of the Sunspots where we have evidence of the presence of water vapour (see Wallace et al. 1995).

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