1997MNRAS.287...79V

Mon. Not. R. Astron. Soc. **287**, 79–86 (1997)

A spectroscopic linelist for hot water

Serena Viti,[1,2] Jonathan Tennyson[1,2] and Oleg L. Polyansky[1]★

[1] *Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT*
[2] *Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA*

Accepted 1996 December 12. Received 1996 December 11; in original form 1996 July 17

ABSTRACT

A new linelist of H_2O transition frequencies and intensities is presented. This list greatly improves the accuracy of the energy levels and the transition frequencies over existing hot water linelists. Although it does not cover many high vibrational states of the molecule, it does include all the rotational levels up to $J=38$. Comparisons with several sets of data (ab initio and experimental) are shown. The accuracy of the linelist should be enough for it to be used to assign laboratory line transitions at high temperature, and to provide water transitions that could be observed in other hot molecular environments including magnetohydrodynamic shocks, circumstellar outflows and active galactic nuclei.

Key words: masers – molecular data – shock waves – Sun: atmosphere – stars: atmospheres – galaxies: active.

1 INTRODUCTION

Water is a complicated but essential molecule for many purposes in astronomy: until a few years ago it was believed to be important only for modelling of cool stars and, of course, of planetary atmospheres. Now it is known to play an important role also in the interpretation of the spectra of sunspots, in the radiative cooling process of the gas in circumstellar outflows, in dissociative and non-dissociative magnetohydrodynamic shocks in dense molecular clouds, in star-forming regions, and finally in extragalactic sources like active galactic nuclei (AGN).

Atlases of M-type stars show that the only unassigned regions of their spectra are the ones dominated by water vapour (Ridgway et al. 1984; Kleinmann & Hall 1986): in fact the modelling of cool stellar atmospheres is made difficult by the many molecular species present in their spectra; in the near-infrared, water is the main source of opacity for cool, solar-metallicity oxygen-rich stars such as the many M dwarfs which dominate 80 per cent of our Galaxy. To model the atmospheres of such stars, it is necessary to cover both high vibrational and rotational states of the water molecule.

Even in stars like the Sun, water plays an important role. Water vapour was identified for the first time in sunspot spectra by Benedict and Hall (Hall 1970); from then onwards, many have attempted the identification of water lines in these spectra (Wallace, Livingston & Bernath 1994; Wallace et al. 1995) using experimental data. In particular, a comparison between the laboratory hot water and sunspot spectra by Wallace et al. led to identification of the majority of the sunspot lines as belonging to water, whereas the specific assignment of these lines to rovibrational quantum numbers has not been done. The problem here is the density of lines, 50 lines per cm^{-1} for example, assignment of which requires calculation of high rotational levels with an accuracy of about 0.01 cm^{-1}.

Hot water is predicted theoretically to be formed in warm post-shock gas in dissociative and non-dissociative shocks in molecular clouds such as those in Orion. At higher temperatures, water is thought to have a dominant role in the cooling process (Draine, Roberge & Dalgarno 1983). Furthermore, Neufeld & Melnick (1987) demonstrated that many far-infrared H_2O rotational transitions are potentially observable. In fact, recent *Infrared Space Observatory* (*ISO*) obervations confirmed the presence of water vapour in star-forming regions like W Hydrae (Neufeld et al. 1996; Barlow et al. 1996).

Theoretical models for physical and chemical conditions in circumstellar outflows predict that large quantities of water should be produced in oxygen-rich outflows (Chen & Neufeld 1995). Finally, over the last 10 years, water maser emission in extragalactic sources has been observed, mainly where nuclear activity is present (Neufeld, Maloney & Conger 1994).

★Permanent address: Institute of Applied Physics, Russian Academy of Science, Uljanov Street 46, Nizhnii Novgorod, Russia 603024.

For analysing, modelling and predicting spectra from all these sources, reliable hot water data are essential.

At present there are few laboratory data on highly rotationally excited (high J) levels in water. The main source of water line parameters is the HITRAN data base which contains 30 117 lines (Rothman et al. 1987; Rothman, private communication). However, HITRAN is limited to rotational bands up to $J=20$, and only includes energy levels up to a maximum of 6000 cm^{-1}, so does not cover high vibrational bands. This and other similar data bases contain many laboratory measurements (see, for example, Flaud, Camy-Peyret & Maillard 1976), but are primarily designed for temperatures of about 300 K. At higher temperatures, many important lines are missing (Schryber, Miller & Tennyson 1995).

Models of cool, oxygen-rich stars such as M dwarfs require extensive data on hot (≥ 2000 K) water (see, for example, Allard et al. 1994, Brett 1995 and Tsuji, Ohnaka & Aoti 1996). These data have been taken from both experimental and computational sources. Experimentally, the Ludwig (1971) steam data are still used for atmospheric modelling and for constructing water band profiles, although these data are too coarse to be useful for the identification of water lines, or indeed reliable modelling (Allard et al. 1994; Schryber et al. 1995). Computationally there are two linelists, due respectively to Jørgensen (Jørgensen 1992; Jørgensen & Jensen 1993, hereafter JJ93) and Miller and Tennyson (Miller et al. 1994; Allard et al. 1994), referred to from now on as MT. The latter contains 6.4 million lines, rotational states up to $J=30$ and energy levels up to 11 000 cm^{-1}.

Recently, synthetic spectra have been produced and used to interpret observations of M dwarfs (Jones et al. 1996). The synthetic spectra tested the two water linelists, JJ93 and MT, and the Ludwig (1971) steam data. All of them failed to reproduce the water molecular bands in the observed spectra. The MT linelist has also been included in the recent non-grey model atmospheres for cool brown dwarfs which have been compared with the coolest dwarf yet discovered, Gl 229b (Allard et al. 1996). However, the energy cut-off of the MT linelist is too low and overall the accuracy of energy levels is not high enough to give a good representation of stellar energy output shortward of about 2 μm (Jones et al. 1995). Spectroscopically also, the MT linelist is of no use. In fact the MT linelist was not designed to be used spectroscopically, and it cannot be used for spectroscopic assignments due to its inaccuracy. HITRAN, on the other hand, although accurate, is insufficient.

More accurate data are definitely needed for both spectroscopic assignments and modelling. Usually spectroscopists use techniques based on perturbation expansions to calculate rotational and vibrational levels close to the ground state (e.g. Flaud, Camy-Peyret & Johns 1983). This involves fitting measured levels using a perturbational Hamiltonian. The parameters obtained from the fit are then used to predict higher unobserved levels. For many molecules that undergo large-amplitude vibrational motion, perturbational expansions of the energy levels become divergent at higher rovibrational energies (Polyansky & Tennyson 1992), and line frequencies calculated from such Hamiltonians may be out by tens or even thousands of cm^{-1}. Among such molecules, water is the classic example.

Alternatively, it is possible to perform variational calculations which show much more reliable extrapolation behaviour (Polyansky, Jensen & Tennyson 1994). Based on work by Tennyson & Sutcliffe (1982), program suites have been developed that calculate energy levels, wavefunctions and dipole transition moments for rotating and vibrating triatomic molecules which, within the Born–Oppenheimer approximation, give variationally exact results for a given potential energy surface. These methods were used to compute the MT linelist, but technical developments (Tennyson & Sutcliffe 1992) and use of more accurate potential energy surfaces (Polyansky et al. 1994) have allowed us to improve significantly the accuracy of these calculations.

With these improvements, we have computed a new linelist (from now on referred to as VTP1) which we present in this paper. VTP1 is somewhere between the two categories discussed above: it is a calculated linelist, it does not cover high vibrational bands, but it does cover high rotational levels. It contains 230 000 lines, much fewer levels than MT; however, it is spectroscopically accurate and it also includes higher rotational levels. The present linelist is designed for spectroscopic analysis, and complements rather than replaces the MT or the JJ93 linelist. VTP1 can be used for studying water spectra, particularly of hot rotational states (Yates, Cohen & Hills 1995). However, it is not complete enough to give opacities for modelling cool stellar atmospheres. The detailed computation of the VTP1 linelist and error estimates are presented in Section 2; comparisons with other linelists and examples of applications are shown in Section 3. The linelist is freely available on-line via ftp or the World Wide Web.

2 COMPUTATION OF THE VTP1 LINELIST

The aim of this work was to compute all the wavefunctions for rotational angular momentum as high as $J=38$, including all the energy levels belonging to the ground vibrational state, (000) ($v_1=0$, $v_2=0$, $v_3=0$). Our final linelist actually includes higher vibrational states and, more specifically, some of the levels for the (000), (100), (001), (011), (010), (021) and (101) states. For high J ($J \geq 10$) we found that it was necessary to consider energies of up to 12 000 cm^{-1} above the ground state.

Water is a triatomic asymmetric top molecule. For an asymmetric top, the total angular momentum J and its projection M on an axis fixed in space are constants of the motions and therefore ‘good’ quantum numbers. There are $2J+1$ sublevels of different energy for each value of J, which can be divided on symmetry grounds into four groups. This is discussed below.

Based on the Tennyson–Sutcliffe approach, two methods have been developed to calculate vibration–rotation wavefunctions: one employs basis set expansions (see Tennyson et al. 1993b). This method was used by Miller et al. (1994) to compute the MT water linelist using the program suite TRIATOM. The second method uses a discrete variable representation (DVR) to calculate wavefunctions on a grid in coordinate space. This method is more efficient for calculating large quantities of data, and it is this method that was used to compute the VTP1 water linelist. Furthermore, theoretical developments (Tennyson & Sutcliffe 1992) mean that the full symmetry of water can be included within a DVR-based approach.

The DVR program suite (Tennyson, Henderson & Fulton 1995) is divided into three programs: DVR3D, ROTLEV3B and DIPOLE.

DVR3D calculates the bound vibrational or Coriolis decoupled rovibrational states using an exact (within the Born–Oppenheimer approximation) Hamiltonian as a starting point to construct the wavefunctions. The kinetic energy operator directly relates the Cartesian positions of the nuclei of a triatomic molecule to a set of internal coordinates comprising two radial coordinates, r_1, r_2, and the included angle, θ. In this work these coordinates are Radau coordinates and the body-fixed axes are taken to bisect the angle [see Tennyson & Sutcliffe (1992) for further details]. We note that the kinetic energy operator used makes no a priori assumptions about the rovibrational separation or equilibrium geometry.

ROTLEV3B performs the second step in a two-step variational calculation for the bound rovibrational levels of a triatomic molecule, giving as an output the energy levels for each angular momentum state J and their wavefunctions.

DIPOLE computes the dipole transition strengths for each transition, using only rigorous, symmetry-based selection rules (see below). An additional program, SPECTRA (Tennyson et al. 1993a), is used to synthesize spectra from the linelist generated by dipole.

For the VTP1 linelist, the energy and wavefunctions were generated using the PJT1 potential of Polyansky et al. (1994). This potential was determined by fits to the spectroscopic data, and is particularly accurate for energy levels belonging to low vibrational states; the observed rotational levels of the ground state are reproduced with a standard deviation of only 0.03 cm^{-1}. However, PJT1 is less accurate for higher states. The dipole transitions were calculated by using the spectroscopically determined dipole surfaces of Wattson & Rothman (1992).

We used a DVR grid of 40 points based on Gauss(associated) Legendre polynomials in the θ-coordinate. For the radial coordinates we used the same radial basis set parameters as MT (see Fernley, Miller & Tennyson 1991) and a DVR grid of 21 points. This number of grid points is sufficient to obtain good convergence for low-lying vibrational levels, but needs extending to converge high vibrational states. In the first vibrational step, we selected 500 eigenvectors out of a 1000-dimensional secular problem (i.e. the maximum dimension of the final Hamiltonian matrix). For the rovibrational problem, the size of the Hamiltonian varied with J as $200 \times (J+1)$. The number of eigenvalues obtained varied with J with no fixed rule. We always ensured that all the energies belonging to the ground vibrational state were included.

The symmetry of water was taken into account by introducing two quantum numbers, p and q, defining respectively the rotational parity and the parity with respect to interchange of the two H atoms. The rotational parity of the system is given by $(-1)^{J+P}$ where $p=0$, 1, and the interchange parity is given by $(-1)^q$ where $q=0, 1$ (Tennyson & Sutcliffe 1992). Our wavefunctions are therefore divided into four symmetry blocks for each rotational angular momentum, J, except $J=0$ for which $p=0$ only. These wavefunctions were used to generate a list of all possible dipole allowed transitions following the rigorous symmetry rules

$$\Delta J=0, \quad \Delta p=\pm 1, \quad \Delta q=0;$$
$$\Delta J=\pm 1, \quad \Delta p=0, \quad \Delta q=0; \qquad (1)$$

The use of properly symmetrized wavefunctions is necessary to account correctly for the nuclear spin statistics. As a conseqeunce, ortho/para doublets very close in frequency have been resolved with the correct intensity ratio; a feature not present in the MT linelist.

It is important to test and estimate convergence and other errors for our calculations before attempting to use the VTP1 linelist for spectroscopic assignments. Self-consistent tests were performed by repeating selected calculations several times for different parameters. These tests suggested that our nuclear motion calculations are converged to higher accuracy than the potential, i.e. 0.3 cm^{-1}, for all levels considered.

An alternative method of checking our results is by comparison with available experimental and theoretical data. We compared the energy levels produced by our DVR method against the ones in the MT linelist and the HITRAN data base (Rothman et al. 1987). In general, the VTP1 levels are a major improvement over the MT energy levels (see Table 1).

It is interesting to point out some of the improvements of the VTP1; over the MT: the MT linelist was calculated with the basis set program suite TRIATOM (Tennyson et al. 1993a) using an older potential energy surface (Jensen 1989) which had a high standard deviation (up to 6.4 cm^{-1}). Moreover, for high rotational states ($J \geq 20$), studies (Polyansky et al. 1994) have shown that Jensen's potential can give errors of up to 30 cm^{-1}. This problem is exacerbated in MT's calculation due to poor convergence at high J (up to 10 cm^{-1}) (Miller et al. 1994). With the DVR method, the convergence is much better and is essentially independent of J.

Table 1. Comparison of sample calculated energy levels with the observed ones from the HITRAN data base. Calculations are VTP1 (this work) and MT (Miller et al. 1994); see text for details.

$\nu_1\nu_2\nu_3$	J	*VTP*1	*Obs*	Obs − Calc	
				*VTP*1	*MT*
010	0	1594.6986	1594.7480	0.0494	1.061
010	1	1618.6243	1618.5590	0.0514	1.061
020	1	3175.6319	3175.4410	0.0136	1.134
100	1	3680.5329	3680.4541	0.0790	1.822
000	2	70.0909	70.0910	0.0001	1.237
010	2	1664.9133	1664.9710	0.0577	1.059
100	2	3750.5293	3750.4639	0.0655	1.821
000	3	136.7620	136.7620	0.0021	1.237
010	3	1731.8466	1731.8979	0.0515	1.074
010	3	1907.6644	1907.6169	0.0484	1.077
001	3	4030.1858	4030.3059	0.1201	1.398
000	4	222.0535	222.0520	0.0015	1.241
010	4	1817.4053	1817.4510	0.0457	1.092
000	11	2144.0347	2144.0470	0.0123	2.850
000	23	5271.4146	5271.3730	0.0416	0.92

Table 2. A sample of output from the VTP1 water linelist.

J''	E''	J'	E'	g	ω	A_{if}
15	7219.7758	16	7219.7664	3	0.00944	$0.29297E-14$
21	9866.5985	21	9866.5702	1	0.02828	$0.17378E-12$
23	8181.6862	22	8181.6307	3	0.05549	$0.10877E-15$
15	9685.0104	15	9684.9441	1	0.06633	$0.55787E-17$
4	1922.8695	5	1922.7950	1	0.07457	$0.56702E-11$
17	9028.4692	18	9028.3509	1	0.11832	$0.23194E-16$
18	8438.5499	19	8438.4201	1	0.12983	$0.13021E-12$
15	6938.8815	14	6938.7360	3	0.14549	$0.15747E-15$
4	3598.7126	5	3598.5495	1	0.16308	$0.14296E-09$
17	9712.2928	16	9712.1121	3	0.18078	$0.45226E-21$
9	2904.6030	10	2904.4189	1	0.18404	$0.48356E-10$
18	9945.7933	17	9945.5767	3	0.21652	$0.15836E-17$
19	8478.8283	18	8478.6024	1	0.22587	$0.91786E-16$
19	8478.8283	18	8478.6024	1	0.22587	$0.91795E-16$
16	9106.8766	16	9106.6499	3	0.22671	$0.17487E-10$
23	7704.5736	23	7704.3268	1	0.24681	$0.28430E-12$
15	9526.0973	16	9525.8396	1	0.25773	$0.62094E-21$
16	9814.7779	16	9814.5087	1	0.26919	$0.47118E-14$
15	9144.5890	15	9144.3109	1	0.27813	$0.57340E-19$
22	6219.8393	21	6219.5360	3	0.30330	$0.17593E-09$
18	6581.2302	17	6580.9125	1	0.31771	$0.14342E-20$
18	6869.0323	17	6868.6956	1	0.33676	$0.31519E-14$
4	1908.0028	3	1907.6644	1	0.33838	$0.60864E-09$
15	5339.8335	15	5339.4940	1	0.33945	$0.75710E-17$
19	6779.2503	18	6778.9063	1	0.34407	$0.22194E-15$
16	8991.2922	15	8990.9471	1	0.34513	$0.19625E-17$
18	6869.0323	17	6868.6843	3	0.34800	$0.34790E-14$
16	9296.4229	17	9296.0269	1	0.39599	$0.31366E-13$
21	7933.5123	22	7933.1111	3	0.40123	$0.61338E-11$
20	9926.8347	20	9926.4118	3	0.42282	$0.39977E-13$
15	3624.1634	16	3623.7184	3	0.44502	$0.42839E-09$
16	8211.1791	15	8210.7222	3	0.45692	$0.34117E-13$
15	9144.5890	15	9144.1100	3	0.47901	$0.53744E-19$
18	9966.8475	18	9966.3058	1	0.54167	$0.11842E-10$
17	8980.9345	16	8980.3901	1	0.54438	$0.85560E-14$
17	9784.1220	16	9783.5577	1	0.56439	$0.25835E-11$
18	8478.6024	17	8478.0151	1	0.58728	$0.71049E-18$
16	7598.8166	17	7598.1900	3	0.62653	$0.65458E-09$
21	8169.4948	22	8168.8335	3	0.66126	$0.23312E-08$
17	6994.0722	17	6993.3780	3	0.69415	$0.72221E-24$
17	8043.7961	16	8043.0837	3	0.71242	$0.67386E-17$
15	6683.0212	14	6682.2770	1	0.74426	$0.41935E-11$
6	447.2549	5	446.5075	1	0.74741	$0.20325E-08$
6	447.2549	5	446.5075	1	0.74741	$0.20325E-08$

Finally, as noted above, MT's TRIATOM calculations used only partial symmetry which did not distinguish between wavefunctions of ortho and para states of water. With DVR, full symmetry of water is taken into account.

Our accuracy tests suggest that errors in our linelist should only be apparent in observations made at a resolving power, $\lambda/\Delta\lambda$, greater than 17 000. However, we note that the tests performed on hot transitions rely on a small sample of lines which have been assigned to the high-temperature laboratory measurements (Polyansky et al. 1996a).

3 RESULTS

Our linelist contains 230 000 lines, which is too many usefully to tabulate here. An illustrative portion of the linelist is given in Table 2. J' and E' are the rotational quantum number and the energy level of the upper state, while J'' and E'' are the corresponding parameters for the lower state. The energies are in cm^{-1}, as is the transition frequency ω $(=E'-E'')$. g is the nuclear spin degeneracy factor, which for water is 1 (para) or 3 (ortho). The Einstein coefficient, A_{if}, is in s^{-1}. It can be used to calculate directly the transition probabilities:

$$|R^2|=\frac{(2J'+1)A_{if}}{(2J''+1)\omega^3};\qquad (20$$

and the integrated absorption intensities depending on the temperature chosen:

$$I=C\frac{\omega g(2J''+1)}{Q(T)}\left[\exp\left(\frac{-E''}{kT}\right)-\exp\left(\frac{-E'}{kT}\right)\right]|R^2|,\qquad (3)$$

where C is the constant of proportionality and is equal to 7.9920×10^{11} for the intensity in cm mol^{-1}, or equal to 3.5656×10^{7} at standard temperature and pressure for the intensity in cm^{-2} atm^{-1}, and $Q(T)$ is the partition function.

The entire linelist is available either via our group World Wide Web page on http://marvin.phys.ucl.ac.uk/home.html or via anonymous ftp to jonny.phys.ucl.ac.uk by looking into the directory pub/astrodata/water/vtp1. The list has been split into 10 files based on frequency in cm^{-1}: for example, file w294 contains transitions from 0 to 294 cm^{-1}, file w587 transitions from 294 to 587 cm^{-1}, and so on.

To demonstrate the use of this linelist, we compare spectra generated from it with spectra generated from other available data. We first calculated the spectrum at room temperature (300 K) and compared it with a spectrum obtained experimentally by Kauppinen, Karkkainen & Kyro (1979). Laboratory data at low temperature are very reliable, therefore a match between calculated and observed spectra at room temperature would confirm the quality of the data. Fig. 1 shows such a comparison: for visual reasons, we have plotted the laboratory measurements in the positive direction, while the calculated spectrum is plotted in the negative direction. The relative laboratory intensities are normalized to match the absolute calculated ones, since the original data were normalized to unity. The match is almost perfect, and certainly falls within the expected error bars. Fig. 2 shows our calculated water spectrum at 300 K compared with the HITRAN data base: again the HITRAN spectrum is plotted in the positive direction. In this case, both sets of intensities are absolute. Figs 1 and 2 show that, at low temperature, the VTP1 linelist is sufficient for assigning water lines and for reproducing the measurements.

There are far fewer data available for comparison at higher temperatures. However, Mandin et al. (1992) published a high-resolution, Fourier-transform flame spectrum with a temperature in the region of 2000 K. A comparison with a water spectrum generated with VTP1 at this temperature is shown in Fig. 3. Mandin et al. made no claims about intensity; indeed, there is a pronounced drop in intensity at the lower end of the spectrum, which is probably due to loss of instrumental sensitivity at these frequencies. In the calculated spectrum there are some missing transitions with respect to the flame spectrum, probably belonging to higher vibrational states. However, the observed line positions are again in good agreement with ours.

Fig. 4 shows the water spectrum at 1000, 2000 and 3000 K.

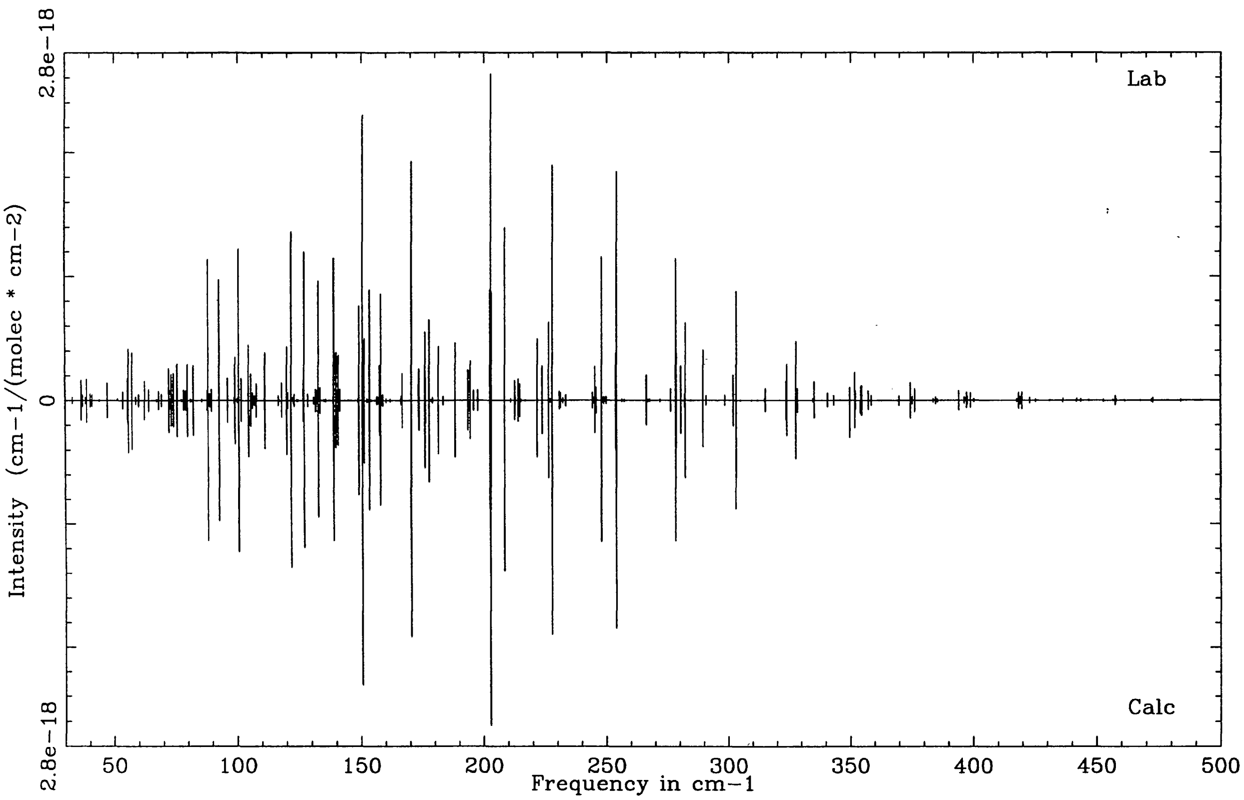

Figure 1. Comparison of the water absorption spectra at $T=300$ K. Upper: laboratory spectrum (Kauppinen et al. 1979); lower: spectrum generated using the VTP1 linelist. The laboratory spectrum has been normalized to the strongest transition in the calculated spectrum.

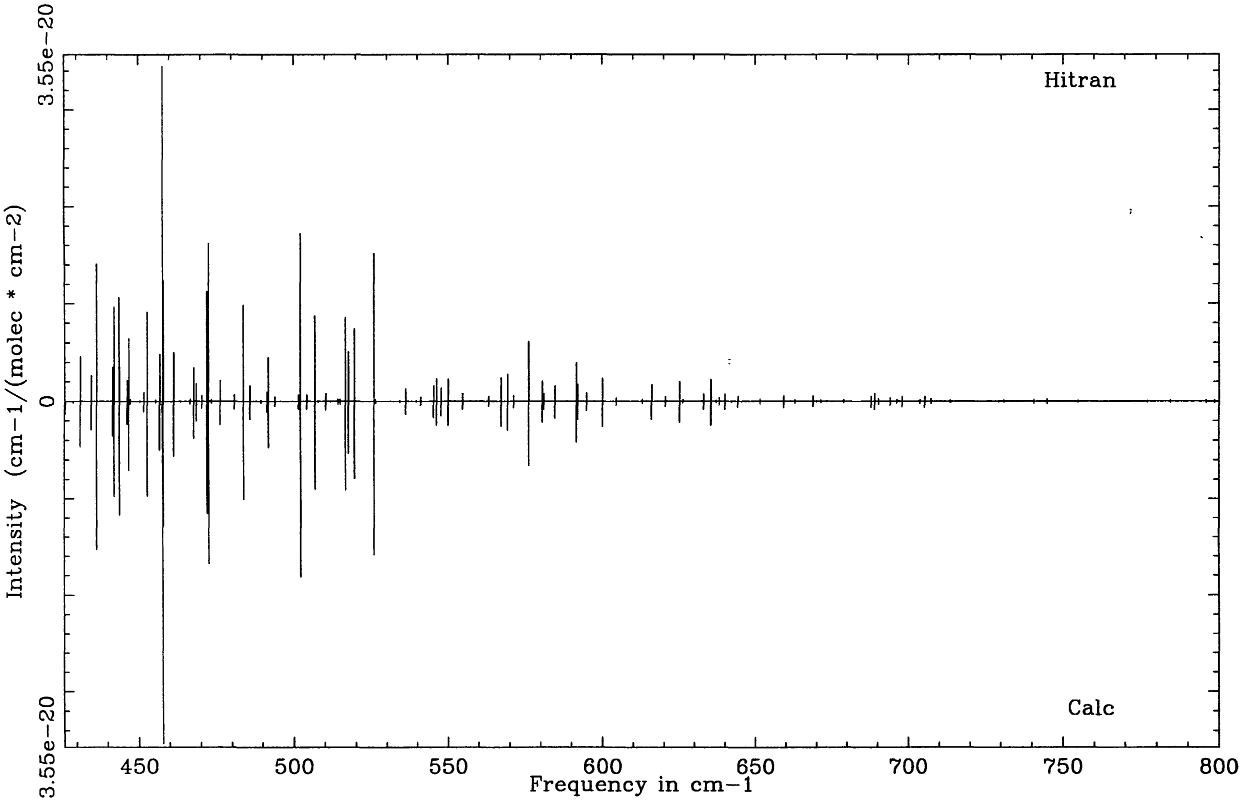

Figure 2. Comparison of the calculated water absorption spectra at $T=300$ K. Upper: generated using the HITRAN data base; lower: generated using the VTP1 linelist.

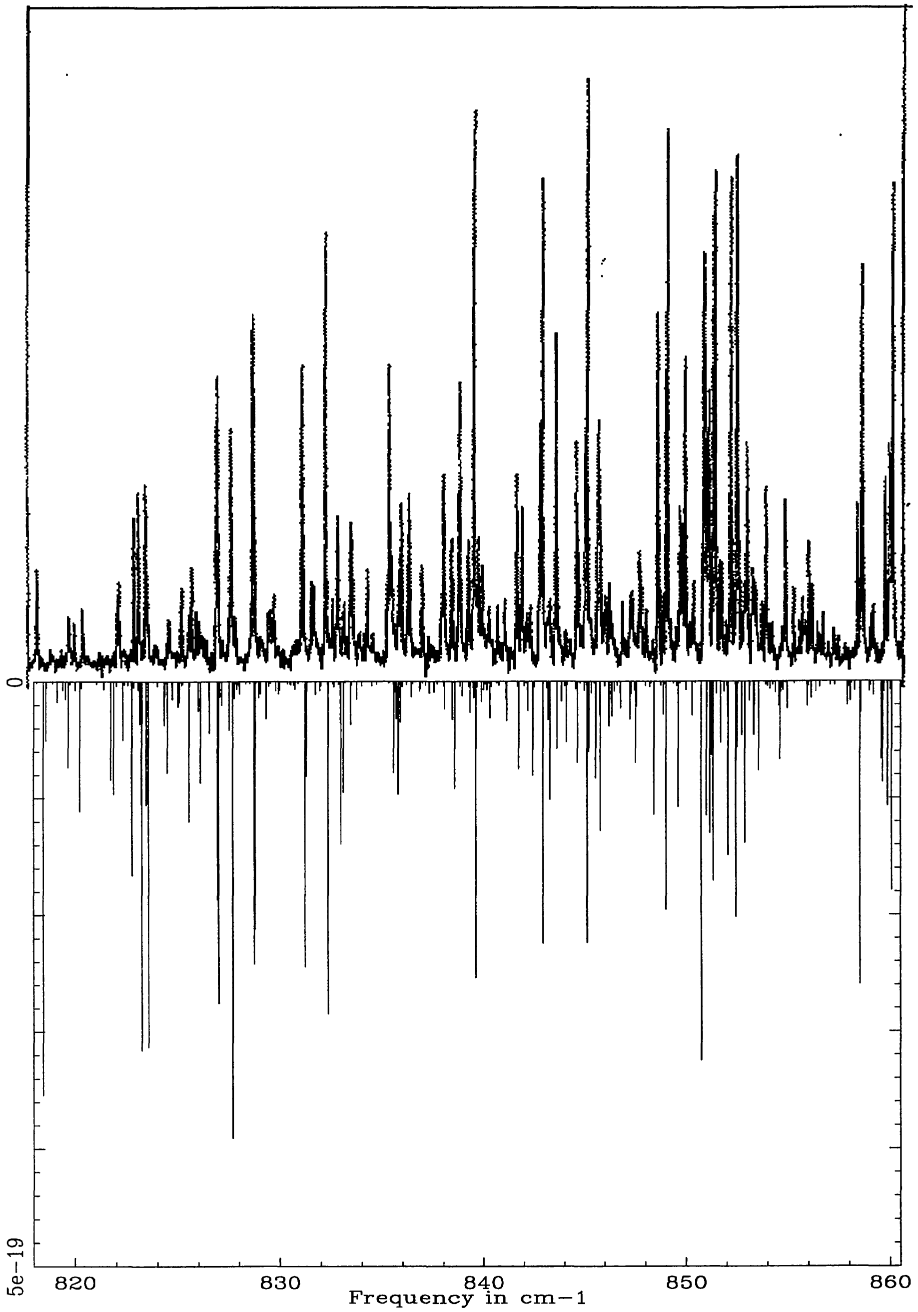

Figure 3. H_2O emission spectrum in the pure rotation band region. Upper: flame spectrum of Mandin et al. (1992) for which the intensity scale is not uniform as a function of frequency; lower: spectrum generated using the VTP1 linelist and $T = 2000$ K; absolute intensities are given in units of cm^{-1} mol^{-1} cm^{-2}.

At high temperature ($T \geq 1000$ K), a significant number of the transitions can be expected to occur among higher vibrational states not included in the list. For this reason, the VTP1 linelist is not sufficient for modelling cool star atmospheres, since these generally weak transitions will still make an important contribution to the opacity. However, we believe that the linelist is complete enough to be used to identify water emission lines in shocked regions of the interstellar medium, in star-forming regions and in masers in AGN.

Finally, we note that since completion of these calculations we have become aware of a new linelist, as yet unpublished (Rothman, private communication), called HITEMP (see discussion in Rothman et al. 1995). The hot water lines in this linelist come from theoretical calculations similar to ours (Wattson & Rothman 1992). We have undertaken some comparisons between the two linelists, and in general we find excellent agreement. For instance, line intensities are the same to within 5 per cent for the cases compared.

4 CONCLUSIONS

We have calculated a water linelist which should have many applications both in astronomy and in molecular spectros-

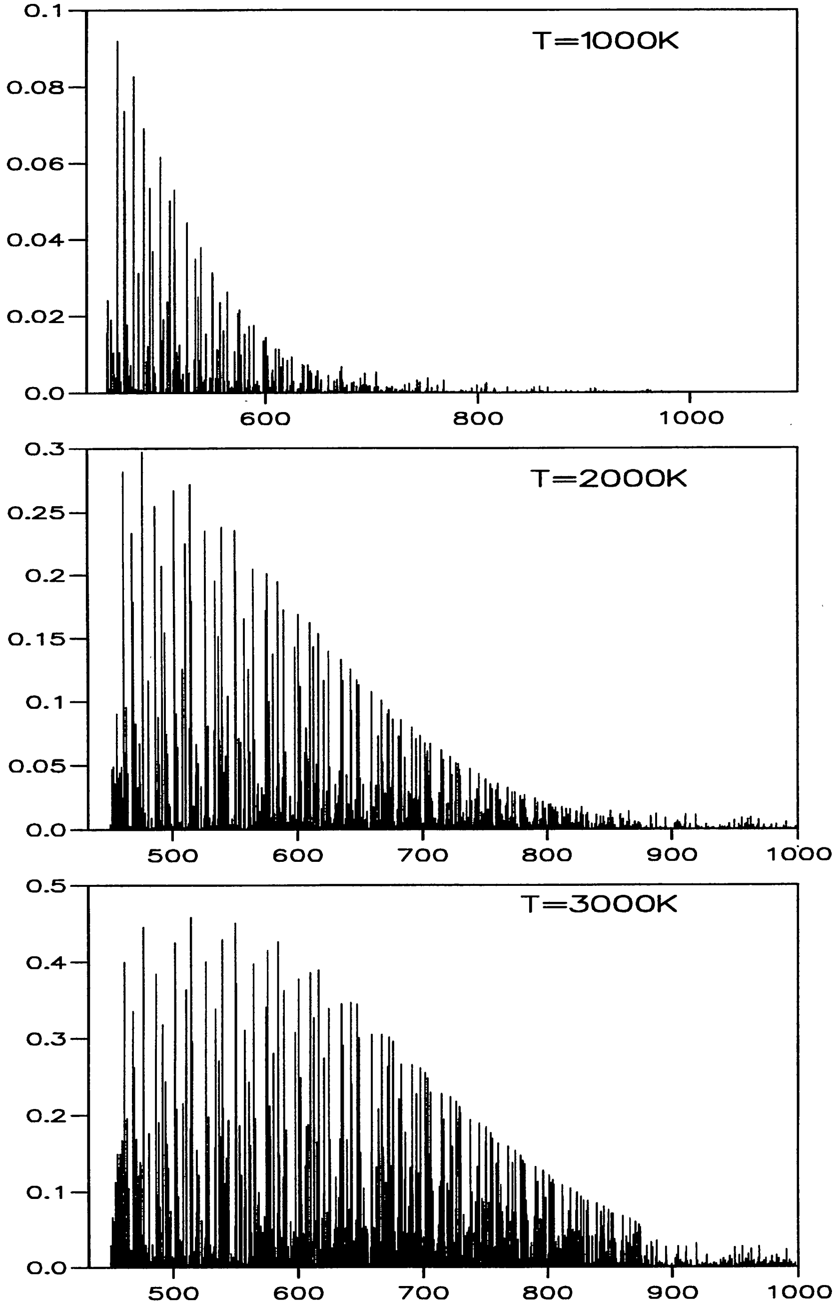

Figure 4. Calculated water emission spectrum as a function of temperature.

copy. We are at the moment using the VTP1 linelist to assign laboratory measurements (see Polyansky et al. 1996a) made at high temperature ($T \sim 1800$ K). So far only about 600 of the strongest lines have been assigned by Polyansky et al., out of about 4000 lines measured. Assignment of laboratory hot water spectra is an important step towards the altogether more challenging task of assigning the many water transitions observed in sunspots.

This work was a major help in preparing a much more complete water linelist, VT2, which will include all the rotational states up to $J=42$ and high enough vibrational states to include levels up to 30 000 cm^{-1} above the ground state. The VT2 linelist will use the new PJT2 potential (Polyansky, Jensen & Tennyson 1996b), which is reliable over a wide range of water vibrational states. It is anticipated that VT2 will be extensive enough to be used for modelling, while VTP1 will continue to be of use in spectroscopic studies. A new linelist for H_3^+ (Neale et al. 1996) has recently been made available; the VT2 linelist, when completed, will also be freely available.

ACKNOWLEDGMENTS

We thank Dr Steven Miller, Dr Liesl Neale and Jeremy Schryber for helpful discussions during the course of this work. We also thank Dr Larry Rothman for supplying data prior to publication. This work was supported by the UK Particle Physics and Astronomy Research Council, the Russian Fund for Fundamental Studies, and the National Science Foundation through a grant for the Institute for Theoretical Atomic and Molecular Physics at Harvard University and the Smithsonian Astrophysical Observatory.

REFERENCES

Allard F., Hauschildt P. H., Miller S., Tennyson J., 1994, ApJ, 426, L39

Allard F., Hauschildt P. H., Baraffe I., Chabrier G., 1996, ApJ, 465, L123

Barlow M. J. et al., 1996, A&A, 315, L241

Brett J. M., 1995, A&A, 295, 736

Chen W., Neufeld D. A., 1995, ApJ, 453, L99

Draine B. T., Roberge W. G., Dalgarno A., 1983, ApJ, 264, 485

Fernley J. A., Miller S., Tennyson J., 1991, J. Mol. Spectrosc., 150, 597

Flaud J.-M., Camy-Peyret C., Maillard J. P., 1976, Mol. Phys., 32, 499

Flaud J.-M., Camy-Peyret C., Johns J. W. C., 1983, Can. J. Chem., 61, 1462

Hall D. N. B., 1970, PhD thesis, Harvard University

Jensen P., 1989, J. Mol. Spectrosc., 133, 438

Jones H. R. A., Longmore A. J., Allard F., Hauschildt P. H., Miller S., Tennyson J., 1995, MNRAS, 277, 767

Jones H. R. A., Viti S., Tennyson J., Miller S., Allard F., Hauschildt P. H., 1996, in Pallavicini R., Dupree A. K., eds, ASP Conf. Ser. vol. 109, p. 717

Jørgensen U. G., 1992, Rev. Mex. Astron. Astrofis., 23, 49

Jørgensen U. G., Jensen P., 1993, J. Mol. Spectrosc., 161, 219 (JJ93)

Kauppinen J., Karkkainen T., Kyro E., 1979, J. Mol. Spectrosc., 71, 14

Kleinmann S. G., Hall D. N. B., 1986, ApJS, 62, 501

Ludwig C. B., 1971, Appl. Opt., 10, 1057

Mandin J.-Y., Dana V., Camy-Peyret C., Flaud J.-M., 1992, J. Mol. Spectrosc., 152, 179

Miller S., Tennyson J., Jones H. R. A., Longmore A. J., 1994, in Jørgensen U. G., ed., Lecture Notes in Physics Vol. 428, Molecules in the Stellar Environment. Springer-Verlag, Berlin, p. 296

Neale L., Miller S., Tennyson J., 1996, ApJ, 464, 516

Neufeld D. A., Melnick G. J., 1987, ApJ, 332, 266

Neufeld D. A., Maloney P. R., Conger S., 1994, ApJ, 436, 127

Neufeld D. A., Chen W., Melnick G. J., de Graauw T., Feuchtgruber H., Haser L., Lutz D., Harwit M., 1996, A&A, 315, L237

Polyansky O. L., Tennyson J., 1992, J. Mol. Spectrosc., 154, 246

Polyansky O. L., Jensen P., Tennyson J., 1994, J. Chem. Phys., 101, 7651

Polyansky O. L., Busler J. R., Guo B., Zhang K., Bernath P. F., 1996a, J. Mol. Spectrosc., 176, 305

Polyansky O. L., Jensen P., Tennyson J., 1996b, J. Chem. Phys., 105, 6490

Ridgway S. T., Carbon D. F., Hall D. N. B., Jewell J., 1984, ApJS, 54, 177

Rothman L. S. et al., 1987, Appl. Opt., 26, 4058

Rothman L. S., Gamache R., Schroeder J. W., McCann A., Wattson R. B., 1995, Proc. SPIE, 2471, 105

Schryber J. H., Miller S., Tennyson J., 1995, J. Quant. Spectrosc. Radiat. Transfer, 53, 373

Tennyson J., Sutcliffe B. T., 1982, J. Chem. Phys., 77, 4061

Tennyson J., Sutcliffe B. T., 1992, Int. J. Quant. Chem., 42, 941

Tennyson J., Miller S., Le Sueur C. R., 1993a, Comput. Phys. Commun., 75, 339

Tennyson J., Miller S., Henderson J. R., 1993b, Meth. Comput. Chem., 4, 91

Tennyson J., Henderson J. R., Fulton N. G., 1995, Comput. Phys. Commun., 86, 175

Tsuji T., Ohnaka K., Aoki W., 1996, A&A, 305, L1

Wallace L., Livingston W., Bernath P. F., 1994, An Atlas of the Sunspot Spectrum from 470 to 1223 cm^{-1} and the Photospheric Spectrum from 460 to 630 cm^{-1}. NSO Technical Report 1994-01, Tucson, AZ

Wallace L., Bernath P. F., Livingston W., Hinkle K., Busler J., Guo B., Zhang K., 1995, Sci., 268, 1155

Wattson R. B., Rothman L. S., 1992, J. Quant. Spectrosc. Radiat. Transfer, 48, 763

Yates J. A., Cohen R. J., Hills R. E., 1995, MNRAS, 273, 529