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Estimate of the $J'J''$ dependence of water vapor line broadening parameters

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ABSTRACT

The dependence of water line broadening coefficients on the "good" quantum numbers – angular momentum and symmetry of the upper and lower levels – is analyzed for rotational quantum numbers up to J=50. Trends are investigated separately for P-, Q-, and R-branch transitions for the atmospherically important isotopologue of water. Results are presented which were obtained using two different methods: By averaging the broadening coefficients from HITRAN-2008 for small J values and also by averaging of data calculated using a semi-empirical method for higher J. The resulting air-broadening coefficients allow water vapor spectra with millions of weak lines to be calculated with an accuracy reasonable for many applications, for example estimation of sun radiation with low resolution. Sample results of calculations are presented.

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1. Introduction

The accuracy of atmospheric radiation transfer calculations remains a serious problem for global climate modeling. The different spectroscopic information used by various authors is a significant source of discrepancies in the calculations of solar radiation absorbed in the atmosphere. One major difficulty concerns the water vapor content of the atmosphere which fluctuates strongly from 0.00001% in the Arctic winter to about 5% (by volume) in the tropics [1]. Water vapor is of particular importance as it is the dominant absorbing component in Earth's atmosphere. According to various estimate water vapor and water in clouds contribute up to 95% of the atmospheric absorption of solar radiation. Thus, a detailed knowledge of water vapor absorption properties is key for modeling of transport of radiation through the atmosphere and climatic change.

In the last few years spectral databases have undergone significant changes due to the rapid development of theoretical and experimental high resolution spectroscopy. In 1999, Lerner et al. made a supposition that the difference between the measured and the calculated atmospheric transmittance may be explained by the absence of weak lines in the standard databases [2]. Later, we demonstrated that neglecting water vapor weak lines influence may be comparable to the influence doubling the content of CO_2 in the atmosphere and may as much as 2 W/m^2 [3–5]. The same conclusion was drawn by Ptashnik [6]. These studies were largely based the 1997 variational water line list of Partridge and Schwenke [7], HITRAN-2000 (2004) [8] and they use simple J dependences to estimate the water line half-widths. However, the 2008 version of HITRAN [9] contains significantly different pressure parameters for water and the new BT2 variational water line list [10] is considerably more extensive than previous ones. In this paper, we present a procedure and results for estimating the $J'J''$ dependence of water line broadening.

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Voronin et al. [11] presented a new set of water data for the 14,395–14,407 cm^{-1} region for calculations of the atmospheric transmission using the exact calculated line parameters and showed that compared to HITRAN, which uses averaged air broadening coefficients, detailed studies can lead to a significant, up to 3% (at resolution 0.001 cm^{-1}), increase of the absorption at long paths through the atmosphere for a zenith angle of 70°. It was found that accounting for all water vapor lines, missing in HITRAN, can contribute up to between 5% and 7% to the absorption in some micro-windows [11]. Chesnokova et al. obtained similar results for the 10,000–11,000 cm^{-1} spectral region [12]; they found that the contribution to the atmospheric transmission of H_2O lines absent in HITRAN calculated with 10 cm^{-1} spectral resolution was up to 1.5% for a vertical path and 4% for a solar zenith angle of 70°.

The issue of obtaining reliable water line parameters in spectroscopic databases such as HITRAN remains an active one and it is known that current parameter are subject to significant uncertainties, particularly regarding their pressure dependence. For this reason we consider here how strong the influence of errors in the broadening half-widths of H_2O lines on the radiation characteristics is likely to be. We compare atmospheric transmission calculations as the H_2O line broadened half-widths increase by 10% for self-broadening and by 1%, 5%, and 10% for air-broadening. The transmission is computed in the 10,000–11,000 cm^{-1} spectral region at slant atmospheric path from 0 to 100 km for "mid-latitude summer" meteo model. The spectral resolution is 10 cm^{-1}.

For a 10% increase in the self-broadened half-widths, the transmission is changed only by 1.6% for a solar zenith angle of 70°, see Fig. 1. For air-broadening, the influence of the uncertainties in the half-width on the transmission calculation is more significant. For a 10% increase in the air-broadened half-widths, we find differences in the transmission of up to 22%, see Fig. 2. For only a 5% error in the air-broadened half-widths the transmission calculation shows an 11% change in the center of 940 nm (10,600 cm^{-1}) band. These uncertainties are important

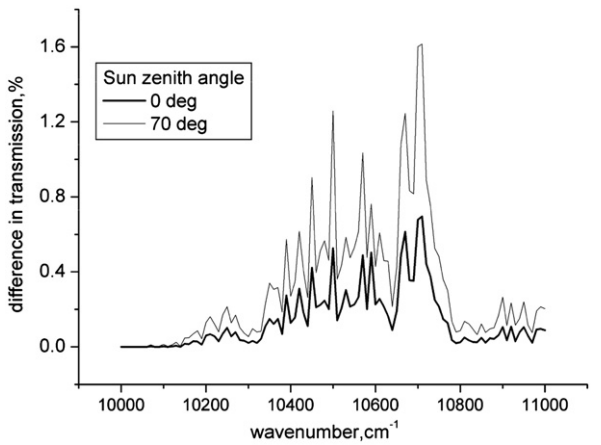

Fig. 1. Influence of a 10% increase of self-broadened half-width of H_2O lines on the atmospheric transmission at different solar zenith angles.

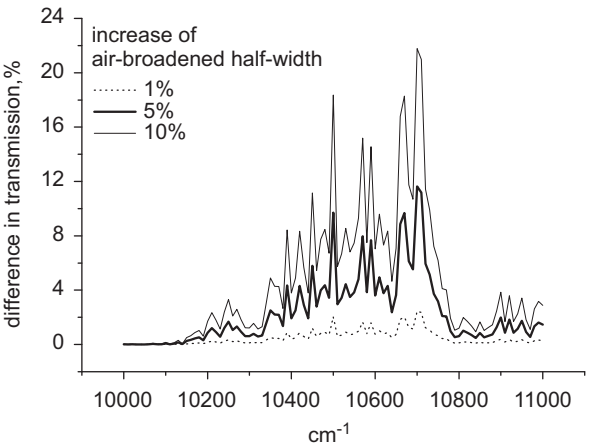

Fig. 2. Influence of an increase in air-broadened half-width of the H_2O lines on the atmospheric transmission at a solar zenith angle of 70°.

for atmospheric models and can potentially lead to large errors in water vapor column retrieval from atmospheric measurements of solar radiation.

The Partridge–Schwenke [7] or BT2 [10] line lists both essentially contain a complete set of water line positions and line strengths but these are labeled only by rigorous quantum numbers and give no pressure-dependent parameters. If either of these line lists is used to augment the line parameters given in databases such as HITRAN, then to be useful for calculating the absorption of solar or other radiation, we need estimates of the broadening coefficients with reasonable accuracy. It is very challenging to calculate the line contour parameters for the say the 508 millions transitions contained in the BT2 line list using modern complicated methods. Besides the huge computer resources needed for such a calculation, only the "good" quantum numbers – angular momentum (J) and symmetry of the upper and lower levels – are available for most transmissions. Approaches for estimating line width parameters have been proposed [13,14], but these require assignments to normal modes (via quantum numbers ν_1, ν_2, ν_3, J, K_a, K_c). Similarly, these quantum numbers are also needed by effective Hamiltonian methods to calculate the matrix elements of the dipole moments of collisionally induced transitions. Recently an alternative method was developed based on the use of a complete set of high accuracy vibration – rotation dipole transition moments calculated for all possible transitions using wave functions determined from variation nuclear motion calculations and an *ab initio* dipole moment surface [15]. This approach explicitly takes into account all scattering channels induced by collisions. However, the calculation of line contour parameters for more than 500 millions transitions using by this approach would take many years.

Therefore, in this work, we present estimated broadening parameters based only on the available J and symmetry quantum numbers. We do in two ways: by averaging the broadening coefficients from HITRAN for small J values and by averaging data calculated using a semi-empirical method for higher J.

2. Estimate of broadening coefficients

2.1. Estimate by averaging the broadening coefficients from HITRAN

The most complete and accurate calculation of centers and intensities of water vapor lines—BT2 [10] contains 508 million transitions for rotational quantum numbers up to J=50. 80% of lines have no quantum number labels such as those which are traditionally used in data banks in normal modes—υ_1, υ_2, υ_3, K_a, K_c. Instead they have only the "good" quantum numbers: J, symmetry and level number.

Attempts to interpolate water vapor half-widths were presented by Gordon et al. [13] and Jacquemart et al. [14]. These authors studied the ro-vibrational dependence of the air-broadened half-widths and the air pressure induced frequency shifts for the $H_2^{16}O$ isotopologue using semi-empirical calculations. Unfortunately, it is not possible to use such an approach to estimate the half-widths for the BT2 line list since the asymmetric top quantum numbers of are missing for most lines.

Calculations of broadening parameters of ro-vibrational lines of molecular gases in the framework of semi-classical theory of Robert – Bonamy (RB) [16] received from the accurate modeling of intermolecular potential and taking into account the subtle details of collisions and intra-molecular dynamics, require the use of complex and long-term calculations even of a single line. That is why the calculations for the whole IR and visible spectral range are extremely laborious. These circumstances lead to the necessity of simplifying the calculation procedure keeping while maintaining accuracy at an acceptable level.

Previously estimates of the weak-line contribution used a linear J-dependence of the broadening [17] obtained by averaging of data from HITRAN-2000 [5]. A more detailed analysis of the rotational dependence of broadening coefficients, conducted on the basis of the analyzing contributions from different intermolecular interaction types and different scattering channels, concluded that the nature of rotational dependence is more complex than it had been considered earlier and revealed its main trends [18]. This analysis makes it possible to predict the values of half-widths basing on asymmetric top rotational quantum numbers—J, K_a, and K_c.

In this work, we calculate the dependency of water lines half-widths on different values of "good" quantum numbers—total angular momentum and the symmetry of upper and lower levels. These dependencies were investigated for different P, Q, and R branches.

To obtain the dependence on rotational quantum number for J up to 20 we used the data from the HITRAN-2008 database. Fig. 3 illustrates J-dependence of the air broadening coefficients taken for the main isotopologue of water. Earlier we performed the same comparison for the data in HITRAN-2004; the resulting curves were within about 1% of those in the figure. We can see the general tendency of the parameters to decrease with the increasing J. The data spread is wide, for example it is from 0.01 to 0.14 cm^{-1} atm^{-1} for J=9, so taking the averaged half-width value for each J is likely to introduce quite significant errors. Fig. 3 also presents the estimates of Ptashnik and Shine [17] and our results.

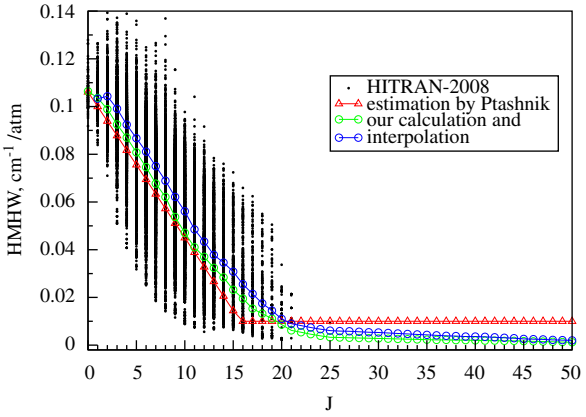

Fig. 3. Dependence of the air broadening coefficient of $H_2^{16}O$ lines on the upper level rotational quantum number J.

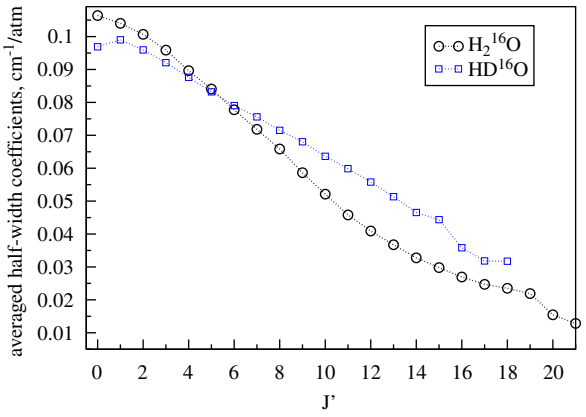

Fig. 4. Dependence on the averaged value of the air-broadening coefficient on the upper level rotational quantum number J' for different isotopologues of water.

Figs. 4 and 5 illustrate the averaged of air-broadening and self-broadening coefficients for two isotopologues of water vapor. Because the pressure-induced values for $H_2^{16}O$, $H_2^{17}O$ and $H_2^{18}O$ isotopologues in HITRAN are essentially identical, only data for the $H_2^{16}O$ and $HD^{16}O$ isotopologues is presented.

Note that there is a significant difference between the air-broadened values for H_2O and HDO, see Fig. 4, but not for the self-broadening coefficients, see Fig. 5.

We note that the figures display some of differences in behavior for $J > 12$. This can be explained by the lack of transitions with large values of total angular momentum in the HITRAN database, so that the resulting averaged values have large statistical uncertainties.

In the BT2 line list symbols 1 – 4 are used to denote symmetry [10]. Allowed transitions are 1–2, 2–1, 3–4, and 4–3. Our investigations revealed that the averaged coefficients for the para 1–2 and 2–1 transitions as well as for the ortho 3–4 and 4–3 transitions are practically identical. Conversely, the division of line broadening

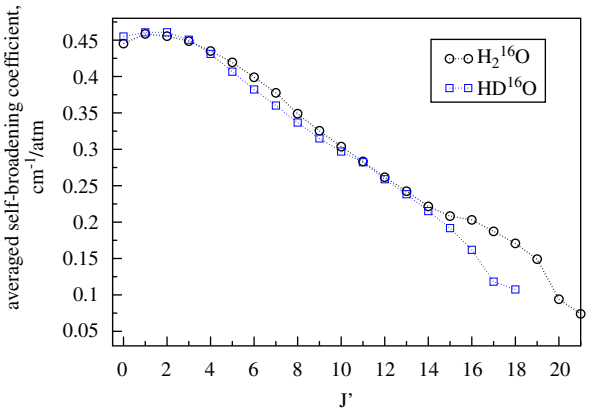

Fig. 5. Dependence of the averaged value of the self-broadening coefficient on rotational quantum number J' for the two isotopologues of water.

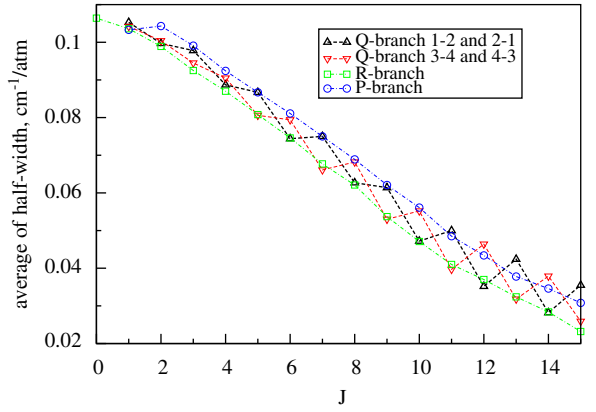

Fig. 6. Dependence of the average value of self-broadening coefficient on the rotational quantum number J' as well as on the branch and the symmetry for $H_2^{16}O$.

coefficients into P, Q, and R branches proved to be quite significant.

Fig. 6 presents six curves for the averaged broadening coefficients depending on the type of the branch and symmetry. One can see that the P and R-branch broadening coefficients hardly depend on symmetry. The case of Q branch is different. In this case for para water (symmetry $1-2$) J even behaves as the R-branch and J odd behaves as the P-branch. For ortho water (symmetry $3-4$) the situation is reversed: J even behaves as the P-branch and J odd behaves as the R-branch. Thus, we can estimate an air-broadening coefficient for any transition of $H_2^{16}O$ with the help of just two curves.

2.2. Estimate by averaging of data calculated using a semi-empirical method, for higher J

In order to obtain the dependence of the broadening coefficients for larger values of the rotational quantum number J, where there is no experimental data for the corresponding lines, we performed calculations within the framework of a previously developed semi-empirical method [18–20] that includes various corrections related to the deviation from the Anderson approximation.

In the framework of semi-classical impact theory, the half-width of the line associated with transition i←f may be written as follows:

$$\gamma_{if} = A(i,f) + \sum_{i'} D^2(ii'|l) P_l^A(\omega_{ii'}) + \sum_{f'} D^2(ff'|l) P_l^A(\omega_{ff'}) + \cdots \tag{1}$$

where $A(i,f) = \frac{n}{c}\sum_2 \rho(2)\int_0^\infty v b_0^2(v,2,i,f)dv$ is a typical summand of the Anderson theory conditioned by an interruption ($b_0(v,2,i,f)$ is the interruption parameter); n is the density of the disturbing molecules, $\rho(2)$ is the buffer molecule levels population, and v is the relative speed of the colliding molecules. The transition strengths $D^2(ii'|l)$ and $D^2(ff'|l)$ related to ii', ff' scattering channels depend solely on the properties of the absorbing molecule and include only the intramolecular effects. The terms with 1=1 is related to the dipole type transitions of the main absorbing molecule. Expansion coefficients $P_1^A(\omega_{ii'})$, also known as the interruption function or the efficiency function, depend on the properties of the absorbing and the disturbing molecules. They depend on the intermolecular potential, the paths of the colliding molecules, the energy level structure and the wave functions of the disturbing molecule. The parameters may be considered as the efficiency functions for the giving scattering channel. $P_1^A(\omega_{ii'})$ is a smoothly changing function so we derive the multiplier to this function without changing the $D^2(ii'|l)$ term that describes the dynamics of an absorbing molecule:

$$P_l(\omega) = P_l^A(\omega)[1 + a_1\omega + a_2\omega^2 + \cdots] \tag{2}$$

where $P_1^A(\omega)$ is the efficiency function in Anderson approximation. The expression in square brackets denotes the corrections for various effects neglected in Anderson theory. Using this form for the efficiency function, calculations of H_2O lines broadening were performed in the following way:

$$P_l\left(\omega_{ff'}\right) = P_l^A\left(\omega_{ff'}\right)\left[c_1/(c_2\sqrt{j_f}+1)\right] \tag{3}$$

where c_1, c_2 are the parameters obtained by the fitting to the experimental values. A feature of these calculations is the use of accurate dipole transition couplings from the BT2 line list [10].

Table 1 presents data obtained by two different methods: (a) by the averaging of HITRAN-2008 data for small values of total angular momentum J ($J<20$). (b) by semi-empirical calculations for large values of J (J=20,…,50). Table 1 shows that the broadening values from the R-branch are close those of the P-branch when $J(R)=J(P)-1$ for J=1,…,14; for higher J's this is not so, which may be due to number of averaged data. Fig. 7 compares of our calculations [15] with experimental data [21]; we can see good agreement for small J values and acceptable one for big J values.

Table 1
Values of air-broadening coefficient for P and R branches of $H_2^{16}O$.

	Air broadening			Air broadening	
J	R	P	J	R	P
0	0.1064		26	0.0032	0.0059
1	0.1036	0.1033	27	0.0031	0.0059
2	0.0989	0.1043	28	0.0030	0.0056
3	0.0925	0.0991	29	0.0029	0.0054
4	0.0870	0.0924	30	0.0028	0.0053
5	0.0808	0.0867	31	0.0027	0.0051
6	0.0746	0.0811	32	0.0026	0.0049
7	0.0677	0.0750	33	0.0025	0.0047
8	0.0621	0.0689	34	0.0024	0.0045
9	0.0537	0.0621	35	0.0023	0.0043
10	0.0471	0.0561	36	0.0022	0.0041
11	0.0410	0.0485	37	0.0022	0.0039
12	0.0370	0.0434	38	0.0021	0.0038
13	0.0324	0.0378	39	0.0021	0.0036
14	0.0285	0.0346	40	0.0020	0.0036
15	0.0232	0.0308	41	0.0019	0.0035
16	0.0195	0.0255	42	0.0019	0.0033
17	0.0153	0.0215	43	0.0018	0.0031
18	0.0132	0.0175	44	0.0018	0.0029
19	0.0111	0.0145	45	0.0017	0.0026
20	0.0086	0.0110	46	0.0016	0.0025
21	0.0062	0.0090	47	0.0015	0.0024
22	0.0054	0.0082	48	0.0014	0.0023
23	0.0046	0.0074	49	0.0013	0.0021
24	0.0039	0.0067	50	0.0012	0.0020
25	0.0033	0.0061			

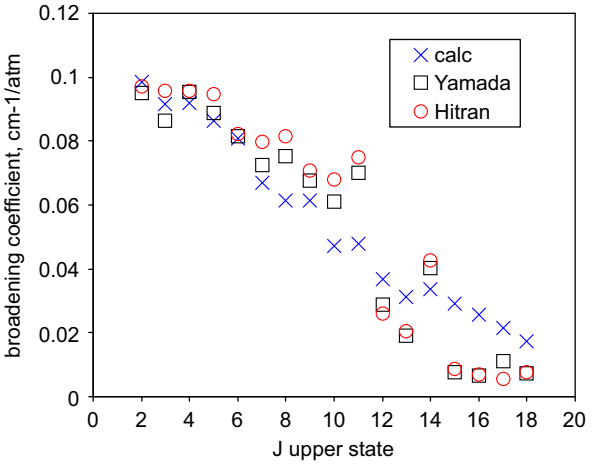

Fig. 7. Dependence of broadening coefficient on rotational quantum number J'. "Calc" is our calculation; "Yamada" is from experiment [21], and "HITRAN" is from the database [9].

3. Discussion and conclusion

To facilitate the use of the BT2 line list with broadening coefficients obtained by the approach presented here, we wrote a code in FORTRAN called "BT2-HW.for". This can be obtained from the web site—http://www.tampa.phys.ucl.ac.uk/ftp/astrodata/water/BT2/HalfWidths, from where the BT2 line list can also be downloaded. This code calculates half-widths using the JJ'-method presented in this paper; the program uses data from output file "fort.36" from program "spectraBT2.for" as the data for input file. The output file "fortHW.36" is of the same format as file "fort.36" except that the half-width coefficient for air-broadening is added to the end of each line. Temperature exponents are generated by code "BT2-HW.for" and presented in the output file "fortHW.36" in the last column. They are calculated according to HITRAN-2004 algorithm (Ref. [8, Table 7]).

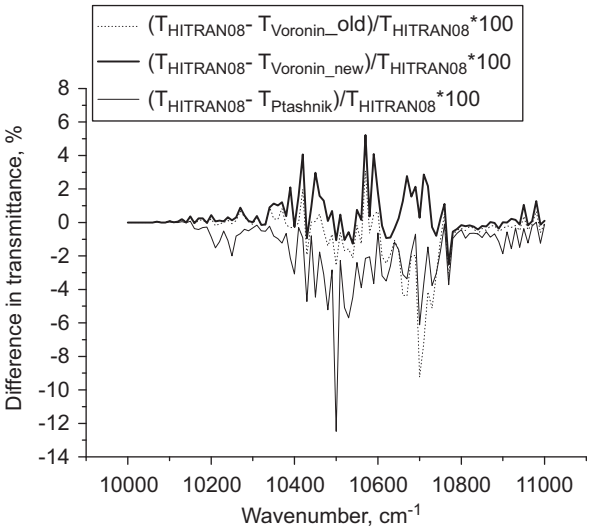

Fig. 8. Relative difference between transmittances, calculated with different air-broadened half-widths from HITRAN-2008, the approximation of Ptashnik and Shine [17], our old data (Voronin et al. [4,5] and the present calculation).

We have calculated the atmospheric transmission of solar radiation with 10 cm^{-1} spectral resolution in the strong H_2O 10,300–10,800 cm^{-1} region using different air-broadened half-widths for the H_2O lines (from HITRAN-2008, approximation [6] and our data [19,20]). The meteorological model is "mid-latitude summer" AFGL [22] with 50 layers from 0 to 120 km. A rapid line-by-line LBL code [23] was used for the calculation of optical thickness of the atmospheric levels.

The relative difference between transmittances, calculated with different air-broadened half-widths (from HITRAN-2008, approximation [17], our old data [4,5] and the present calculation) is shown in Fig. 8. For this comparison we include only those transitions given in HITRAN. The maximum difference between transmissions, calculated with our half-widths and those from HITRAN, is 5.5%, whereas maximum difference between transmissions, calculated with approximation method [17] and HITRAN, is 13% in this spectral region.

Using our observed regularities in the water line broadening coefficients, we can calculate water vapor spectra that include millions of weak lines with reasonable accuracy. The importance of such calculations is demonstrated by the presence of experimental data for large values of rotational quantum number J obtained in hot spectra [24] (the ground vibrational state 000, J=42, states 010, J=39 and 020, J=36). Data for even larger

values of J are present in theoretical studies: the BT2 $H_2^{16}O$ line list [10] contains transitions involving J up to 50, while Partridge and Schwenke's line list [7] considers J up 55. As an illustration of the use of the present estimates, they have been used to construct water monomer line lists for the analysis of broad-band, long path length absorption by water vapor at elevated temperatures Fig. 9 compares how our line list performs compared to HITRAN-2008. These studies were aimed at characterizing possible absorption by the water dimer and it was found that the analysis depended strongly on the use of augmented line lists which employed the broadening coefficients presented here; full details of this work will be presented elsewhere [25] which includes a detailed comparison with new, long path length experiments.

Finally we note that water an important in astrophysical molecule; it is found in a large variety of objects including comets, sunspots, brown dwarfs, M-dwarf stars and planetary atmospheres, both solar and extra-solar. The BT2 line list has become increasingly important as a source of water data for modeling both the opacity and spectra of all these objects. For several of these cases it would be desirable to add line contour parameters, complete with their temperature dependence. The present approach can be very effectively extended to broadening by gases important planetary and stellar atmospheres such as He or H_2. The data for broadening by these species are not that abundant, and, in particular, there is a lack of data with high J transitions. A procedure based on averaging broadening parameters as a function of J and symmetry quantum numbers does not give such a clear picture for these species, compared to cases as where we have a huge data set such as from HITRAN. However it should be possible to use in the trends identified in this work broadening by species such as He, Ar, or H_2.

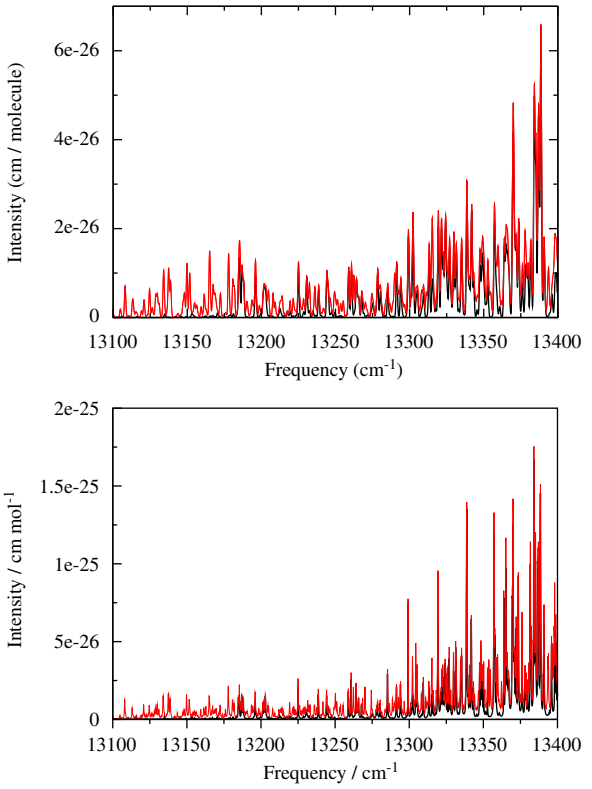

Fig. 9. . Comparison of simulated absorption spectra for pure water vapor generated using HITRAN-2008 (lower curves) and HITRAN-2008 augmented with lines from the BT2 line list and line widths from this work. Upper figure, T=296 K; lower figure, T=373 K.

Acknowledgments

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