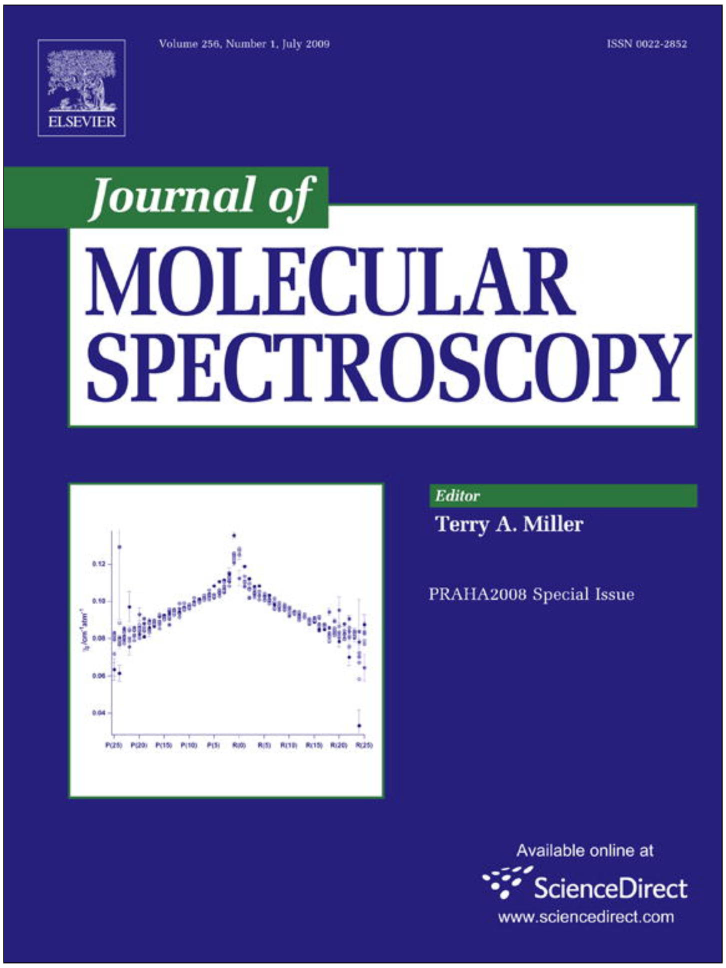
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Calculation of solar radiation atmospheric absorption with different H_2O spectral line data banks

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ABSTRACT

A comparison of the atmospheric absorption calculated with different data banks of water vapour absorption lines is made. The HITRAN database, Barber-Tennyson line list (BT2), calculation of Partridge and Schwenke (PS) are considered. The contribution of H_2O lines, absent in HITRAN, to the atmospheric transmission, calculated with 10 cm^{-1} spectral resolution in the 10000–20000 cm^{-1} spectral region is up to 1.5% for a vertical path and 4% for a solar zenith angle of 70 deg. The highest difference is observed in the 940 nm band. The incoming fluxes of solar radiation, measured by a rotating solar spectroradiometer, were modeled with BT2 and HITRAN database. The difference between measured and calculated fluxes does not exceed the instrumental uncertainties.

1. Introduction

At present there is a discrepancy between measured and calculated fluxes of solar radiation at the Earth's surface. This discrepancy correlates with column density of water vapour. According to our previous investigation [1], the calculated contribution of numerous weak water vapour absorption lines, which are usually ignored in the atmospheric radiation problems, to irradiance of the Earth's surface can reach 2 W/m^2. Similar conclusions have been reached in other studies [2,3].

Many atmospheric experiments use spectroscopic techniques to retrieve the H_2O concentration from the atmospheric radiative fluxes. These methods require accurate knowledge of reference information about spectral line parameters. The spectroscopic data banks are regularly updated. And we made a comparison of the atmospheric absorption calculated with different data banks of water vapour absorption lines. We consider the impact of the difference between H_2O line parameters in the HITRAN database [4,5], Barber-Tennyson line list (BT2) [6], calculation of Partridge and Schwenke (PS) [7], and the recalculated PS data presented as part of SPECTRA [8] on the calculation of the atmospheric absorption of solar radiation.

2. Water vapour data banks

The HITRAN [4,5] is the most popular spectroscopic database for atmospheric radiative calculations. HITRAN relies substantially on laboratory measurements and is regularly updated as better measurements become available. In particular nearly all the data on $H_2{}^{16}O$ was updated between the 2001 and 2004 releases of the database. The most recent available version of the HITRAN water data is via the HITRAN website [5]. This version, which is referred to as HITRAN2006 below, has improved air-broadened half-widths for water and an update for the $H_2{}^{17}O$ and $H_2{}^{18}O$ isotopologues; HITRAN2006 contains the same $H_2{}^{16}O$ lines as HITRAN2004.

The PS data bank [7] was produced on the basis of high accuracy ab initio calculation by Partridge and Schwenke. It contains more H_2O lines than HITRAN.

The list, BT2[6], was calculated using a discrete variable representation two-step approach for solving the rotation-vibration nuclear motions [9]. It is the most complete water line list in existence, comprising over 500 million transitions (65% more than any other list). At atmospheric temperatures, some transitions have extremely weak intensities (10^{-99} cm/molecule). These lines are not included in current versions of spectroscopic databases HITRAN and GEISA and usually not taken into account in atmospheric radiation modelling.

The number of $H_2{}^{16}O$ lines in the data banks is shown in Table 1. BT2 line list is 8000 times greater than HITRAN and about 800 times greater than PS in the spectral region from 9000 to 20000 cm^{-1}. It can be seen, that the number of strong lines, included in HITRAN database, is limited, but the number of weak lines grows rapidly with the decreasing line strength. For extremely weak lines with intensities less than 10^{-80} cm/molecule the line number decreases, but this is only the effect of calculation truncation. All calculations were limited to rotational quantum number J = 50 or less. To estimate the actual numbers of these, extremely weak lines one needs to make calculation up to dissociation energy.

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Table 1
The number of $H_2^{16}O$ lines in the different spectroscopic data banks.

Spectral interval (cm^{-1})	Spectral line data bank		
	BT2 [6]	PS [7]	HITRAN2004 [4]
9000–10000	20825195	10675	554
10000–11000	17774321	18654	2742
11000–12000	15010019	10862	711
12000–13000	12588904	12866	1031
13000–14000	10480937	15622	1720
14000–15000	8588504	12284	1528
15000–16000	6977227	12835	1516
16000–17000	5606762	11689	1118
17000–18000	4423476	12502	1061
18000–19000	3430768	11053	712
19000–20000	2613454	9647	704
9000–20000	108319567	138689	13397

Fig. 1 presents the number of $H_2^{16}O$ lines for each decade of line intensity. We can see that the most of the BT2 lines that are not included in HITRAN, are weak. Our preliminary estimation shows that the lines with intensities higher than 10^{-35} cm/molecule cannot be neglected in atmospheric calculations. In the atmospheric transmission calculation we take into account the lines from BT2 list with intensities higher than 10^{-40} cm/molecule.

3. Atmospheric absorption calculation

We compared H_2O lines from HITRAN2006, the latest update on the HITRAN website [5], and other H_2O data banks: BT2 for $H_2^{16}O$ [6]; $H_2^{17}O$, $H_2^{18}O$ (quantum numbers $J > 10$) calculation by Partridge and Schwenke [7]; $H_2^{17}O$, $H_2^{18}O$ (quantum numbers $J \leqslant 10$) calculation by program DVR3D [9,10]; HDO data [11]. Lines were assumed to be identical, if the following parameters coincide: quantum numbers, transition frequency, and lower energy level. We identified lines absent in HITRAN, and then used them in our calculations.

For the atmospheric application one also needs the line broadening parameters. At the present time such data for weak lines is not available and so they must be determined. The dependence of the H_2O line broadening coefficients on the quantum numbers was analyzed over a wide range of J quantum numbers up to 50. The dependencies were studied for different branches P, Q, R. The required data were obtained in two different ways: by averaging the broadening coefficients from HITRAN2006 for small J values and by averaging semi-empirical data [12,13] for high J (up to 50). After some analysis it was found that calculated linewidths [12,13] allow one to perform calculations with reasonable accuracy for the millions of weak lines.

We have calculated the atmospheric transmission with 20 cm^{-1} spectral resolution for "mid latitude summer" from 0 to 100 km. Air and self broadened halfwidths are calculated from J-dependent H_2O spectra [12,13]. Line shifts were ignored because of the large spectral resolution used in the calculations. The contribution of

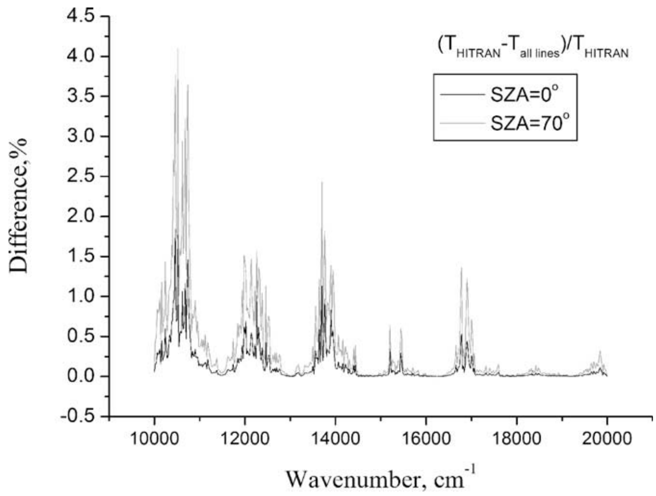

Fig. 2. Contribution of H_2O lines, absent in HITRAN, to the atmospheric transmission at the different solar zenith angles.

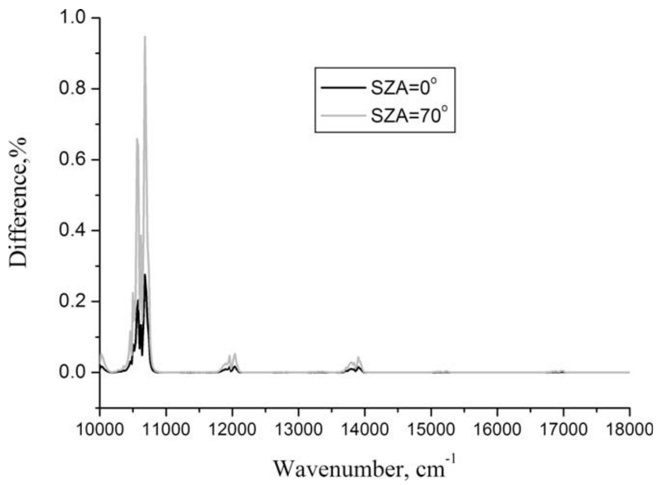

Fig. 3. Contribution of HDO lines, absent in HITRAN, to the atmospheric transmission at the different solar zenith angles.

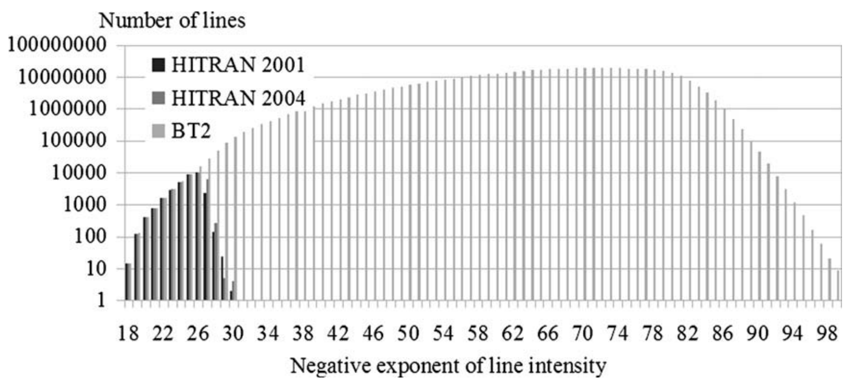

Fig. 1. Number of $H_2^{16}O$ lines for an order of changing line intensity values for temperature 296 K.

H_2O lines, absent in HITRAN, to the atmospheric transmission is up to 1.5% for a vertical path and 4% for a solar zenith angle of 70 deg. (Fig. 2). The highest difference is observed in strong bands such as 940 nm (10 640 cm^{-1}) band.

A contribution of HDO lines, absent in HITRAN, to the atmospheric transmission is presented in Fig. 3. It reaches 1% for a long atmospheric path. It is to be expected that HDO should be more important than the other minor isotopologues of water, despite of its low abundance since the bands of HDO are significantly shifted from those of $H_2{}^{16}O$ and hence HDO absorbs in atmospheric windows.

The difference between the atmospheric transmissions, calculated with BT2[6], HITRAN2006 database [5], PS data, taken from the spectra.iao.ru of the IAO site [8] and initial PS calculation of 1997 [7] for the 940 nm band is shown in Fig. 4. There are large discrepancies between transmissions even for 10 cm^{-1} spectral resolution and vertical atmospheric path. In particular this figure shows the significant improvement given by the recalculation [8] compared to the original PS data [7].

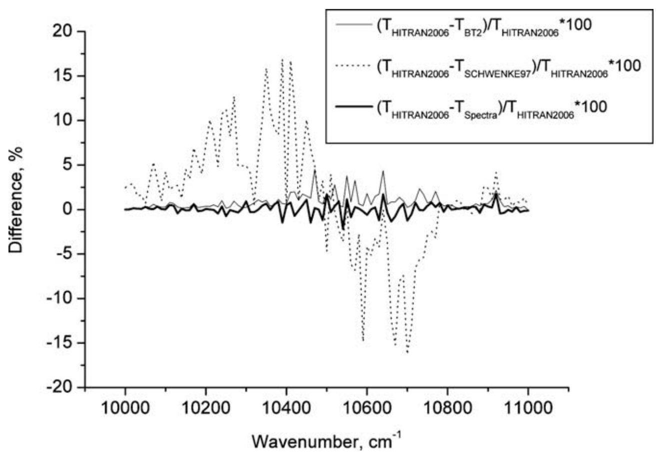

Fig. 4. The difference between the atmospheric transmissions, calculated with BT2 [6], HITRAN2006 [5] database, PS data, taken from the spectra.iao.ru of the IAO site [8] and initial PS calculation of 1997 [7] for "mid latitude summer" meteo model and vertical path. Spectral resolution is 10 cm^{-1}.

4. Comparison of simulated and measured incoming solar fluxes

One of the methods often used to retrieve optical characteristics of the atmosphere is the method based on interpretation of downward solar fluxes measurements at the Earth's surface. To estimate the effect of difference of H_2O spectral line parameters in modern data banks, we have performed numerical simulation of the operation of a solar spectroradiometer with BT2 and HITRAN databases and compared with measurements data.

The data on the spectral fluxes were obtained with the Rotating Shadowband Spectroradiometer (RSS), which measures the direct, diffuse, and net radiation in 512/1024 channels within the optical region (350–1075 nm) [14]. The vertical profiles of the pressure, temperature, and water vapour were retrieved from radiosonde data, while the liquid water path of clouds was retrieved from the data of microwave sensing. The top and bottom boundaries of the cloud layer were determined with the aid of ground-based radars. The calculations accounted for the spectral behavior of the surface albedo derived from the MFRSR (Multi-filter Rotating Shadowband Radiometer) measurements [15] and a rural aerosol, visibility range of 23 km. The cloud extinction coefficient was chosen so that the calculated and measured spectral fluxes coincided in the 500–550 nm band. The effective radius of cloud droplets varied in the range from 6 to 11 μm and corresponded to the typical values of stratus clouds in the region under study [16]. (The data were kindly presented to us by Z. Li, A. Trishchenko, and M. Cribb, Canadian Cen-

Table 2
Atmospheric parameters used as input data in calculations of spectral sunlight fluxes; experiments were conducted as Atmospheric Radiation Measurement Southern Great Plains site (USA).

Date	Solar zenith angle (deg.)	Total content (cm)			Position of the cloud layer (km)	Cloud optical depth at 550 nm	Effective radius (μm)
		Water vapour	Liquid water	Ozone			
October 19, 1997	47.15	1.6	0.008	0.34	0.58–0.85	16.5	7.2
August 05, 1998	24.39	4.1	0.019	0.33	1.49–1.88	25.9	9.1

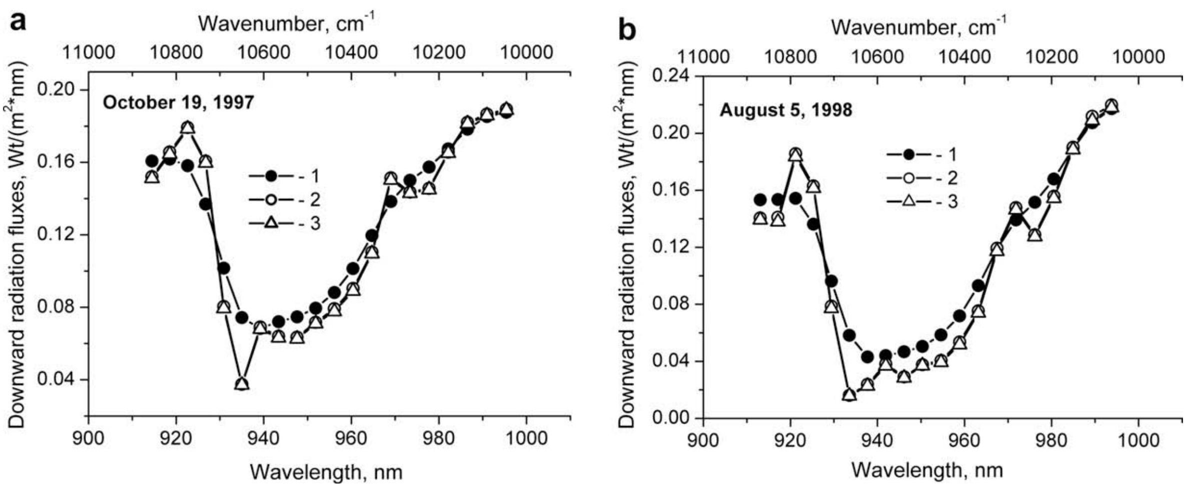

Fig. 5. RSS measurements (curve 1) of downward sunlight fluxes at the Earth's surface for the cloud situation of October 19 of 1997 (a) and August 5 of 1998 (b) compared to our calculations using HITRAN2006 (curve 2) and BT2 (curve 3).

tre for Remote Sensing, Ottawa, Canada [17,18]). It is assumed that the reference model RSS filters profile, closest to the real one, is well approximated by the truncated Gaussian function [19].

The effective absorption coefficients were calculated using the HITRAN2006 [5] database and BT2 line list. The *k*-distribution method [20] was used to shorten the time of calculation of the spectral fluxes taking into account absorption in the spectral ranges determined by the characteristics of filters. The values of the extraterrestrial solar constant were taken from [21,22].

We have calculated the spectral fluxes in the 900–1000 nm (10000–11100 cm^{-1}) band for two different situations, see Table 2, using the algorithm described in detail in [23]. The aerosol characteristics corresponded to the cont-I model of the continental aerosol. Scattering in clouds was simulated using the Heney–Greenstein scattering phase function.

The comparison simulated and measured fluxes showed that in all cases considered our calculation are in a satisfactory agreement with experimental data, see Fig. 5. Furthermore, the fluxes, calculated with BT2 and HITRAN2006, are identical.

5. Conclusion

The H_2O weak lines contribution is essential for microwindows, long atmospheric paths and the hot atmospheres of planets and can not be neglected in the atmospheric absorption calculation.

Contribution of H_2O lines, absent in HITRAN, to the atmospheric transmission, calculated with 10 cm^{-1} spectral resolution in the 10000–20000 cm^{-1} spectral region is up to 1.5% for a vertical path and 4% for a solar zenith angle of 70 deg.

The contribution of HDO lines, absent in the current edition of HITRAN, to the atmospheric transmission, calculated with 20 cm^{-1} spectral resolution, reaches 1% for a long atmospheric paths.

Atmospheric downward fluxes of solar radiation, calculated with BT2 and HITRAN06 in the 900–1000 nm (10000–11100 cm^{-1}) spectral region, give satisfactory agreement with the experimental data.

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