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Notes

Collisional broadening and shifting of the 2_{11}-2_{02} transition of $H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$ by atmosphere gases

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ABSTRACT

Broadening and shifting of the 2_{11}–2_{02} transition of $H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$ by pressure of water, nitrogen and oxygen were precisely measured at room temperature using spectrometer with radio-acoustic detection of absorption. Shift parameters for all studied lines as well as broadening parameters of $H_2{}^{17}O$, $H_2{}^{18}O$ lines were measured for the first time. Comparison of obtained results with previously known experimental and theoretical data is presented.

Submillimeter wave water lines play an important role for atmospheric applications, in particular for remote sensing of the Earth's atmosphere. Laboratory measurements of spectroscopic parameters of the diagnostic lines (intensity, broadening and shifting) are crucial for retrieval of atmospheric parameters from remote sensing data. One line parameters measured using different techniques and methods of study could be significantly different. In this case only multiple measurements of the line parameters by different technique can provide its real accuracy and reliability and meet modern requirements on spectroscopic data precision for atmospheric applications.

By this paper we continue a series of our studies of water lines in millimeter and submillimeter ranges [1–3]. Present study is devoted to room temperature measurements of collisional broadening and shift parameters of pure rotational transition 2_{11}-2_{02} in the ground vibrational state of $H_2{}^{16}O$ at 752.033 GHz, $H_2{}^{17}O$ at 748.458 GHz and $H_2{}^{18}O$ at 745.320 GHz. The experiment was carried out using BWO-based spectrometer with radioacoustic detector (RAD spectrometer). The details of apparatus and methodology of water lines measurements used are given in Refs. [3,4]. Some experimental conditions such as path lengths and partial pressures of water, nitrogen and oxygen as buffer gasses are presented in Table 1. Double distilled water sample as well as high purity (better than 99.99%) nitrogen and oxygen were used. The sample pressure in the gas cell was controlled by MKS baratron pressure gauge (Type 627-B of 10-Torr range) with a declared accuracy of 0.12%. All measurements were performed at 297 ± 1 K.

Table 1
Experimental conditions used in this study.

Line	Perturbing molecule	Path length (cm)	Partial pressure (Torr)	
			H_2O	N_2/O_2
752 GHz $H_2{}^{16}O$	H_2O	1.75	0.4–2.55	–
	N_2/O_2	1.75	0.02	0.4–4.0
748 GHz $H_2{}^{17}O$	H_2O	20	0.4–2.2	–
745 GHz $H_2{}^{18}O$	H_2O	20	0.5–2.0	–
	N_2/O_2	20	0.12–0.3	0.4–2.6

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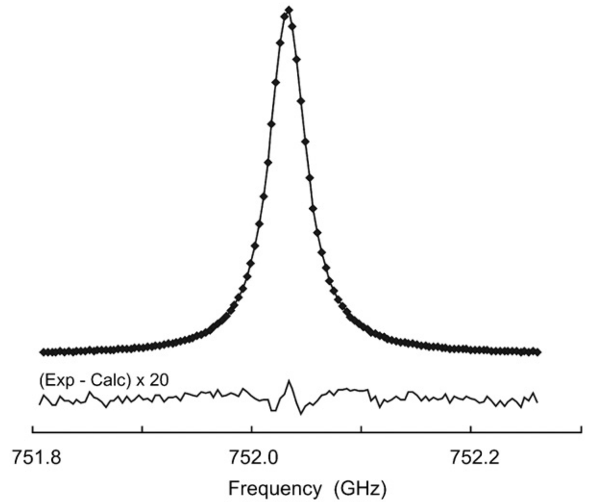

Fig. 1. Experimental record of the 752-GHz water line (diamonds) at 0.85 Torr of H_2O in the cell and its fit by Voigt profile (solid line). The (Exp.-Calc.) residual of the fit magnified as noted is shown in the lower part.

The Voigt line shape was used to extract line parameters from experimental record. An example of the line shape fit result is shown in Fig. 1 for the 752-GHz $H_2{}^{16}O$ line. The magnified residual of the fit is shown in the lower part of the figure. The typical pressure dependences of collisional line width (HWHM) and center position of the 752-GHz line are presented in Fig. 2. Corresponding pressure broadening and shift parameters were obtained as a slope from the result of linear regression of the experimental data.

The results of our measurements are collected in Table 2 as well as previous experimental [5–7] and theoretical values [8]. The present study uncertainties given in parentheses are one standard deviation in units of the last digit quoted. To our knowledge, the experimental investigation of collisional parameters for the 745 and 748-GHz lines as well as shift parameters for all the lines studied were carried out for the first time.

Broadening and shift parameters of the water 2_{11}-2_{02} transition measured in the present study for different water isotopologues coincide with each other within the experimental errors. The same similarity of the parameter

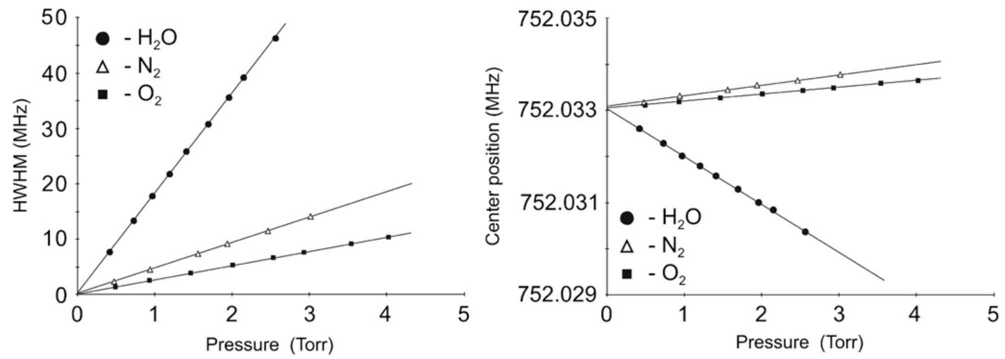

Fig. 2. Experimental pressure dependences of HWHM (left) and center position (right) of the 752-GHz water line for H_2O (●), N_2 (Δ) and O_2 (■) as buffer gases. Solid lines are results of linear regression of the experimental data.

Table 2
Center position (MHz), broadening and shift coefficients (MHz/Torr) of water 2_{11}-2_{02} transition lines by pressure of atmospheric gases (T=297 ± 1 K).

Line	Gas	Center, MHz	Broadening, MHz/Torr	Shifting, MHz/Torr	Reference
752 GHz $H_2{}^{16}O$	H_2O	752033.113(14)	18.110(150)	− 1.170(30)	Present study
	N_2		4.580(50)	+0.235(30)	Present study
			4.450(48)		[6]
			4.16(18)		[7]
			4.552	+0.248	[8] theory
	O_2		2.540(30)	+0.145(15)	Present study
			2.136(64)		[6]
			2.569	+0.161	[8] theory
	Air[a]		4.152(46)	+0.216(27)	Present study
			4.50(16)		[9]
748 GHz $H_2{}^{17}O$	H_2O	748458.660(65)	18.130(450)	− 0.890(300)	Present study
745 GHz $H_2{}^{18}O$	H_2O	745320.180(40)	18.120(130)	− 1.125(140)	Present study
	N_2		4.450(100)	+0.245(60)	Present study
			4.434	+0.250	[8] theory
	O_2		2.550(55)	+0.150(40)	Present study
			2.514	+0.169	[8] theory
	Air		4.051(91)	+0.225(56)	Present study

Uncertainties given in parentheses are in units of the last digit quoted; in this work it corresponds to one standard deviation.
[a] X_{Air}=0.79 X_{N2}+0.21 X_{O2}, X – broadening or shifting parameter.

values for non-deuterated water isotopologues follows from theoretical calculations of Gamache [8] performed using the complex Robert–Bonamy (CRB) formalism. The coincidence of present study values and theoretical results of Ref. [8] proves high accuracy and reliability of both experiment and theory. Measured foreign-broadening parameters for the 752.033-GHz line are also in general agreement with previous data [6,7,9]. However, the discrepancy between these parameters is somewhat higher than quoted experimental uncertainties and could arise from systematic errors of experiments that are usually hard to reveal and take into account.

Earlier study of the submillimeter wave water lines up to 5 THz performed by Matsushima [5] gives rest frequency of the 2_{11}-2_{02} transition $H_2{}^{16}O$ line as 752033.104(13) MHz. This value does not take into account the line self-shift and could be slightly corrected using present study self-shift parameter and pressure 4.7 Pa from Ref. [5]. The corrected center 752033.145(14) MHz is in good agreement with value 752033.113(14) MHz from Table 2 proving consistency of measured line center and its shifting.

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