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Analysis and analytical modeling of Air, N_2, O_2 and CO_2 broadening coefficients of Water Vapor Lines in the 380−26000 cm^{-1} Spectral Range

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The analysis of the available experimental data on the H_2O line broadening coefficients by air, nitrogen, oxygen and carbon dioxide in the spectral range 380−26000 cm^{-1} is carried out. The analysis is based on the application of the analytical model $\gamma(sur)$, which depends on the fitting parameters. $N = 4110$, $N = 757$, $N = 658$ and $N = 688$ air, nitrogen, oxygen and carbon dioxide broadening coefficients derived from the fitted parameters agree with measurements with an average accuracy of 7.2%, 11.6%, 7.6% and 7.1%, respectively. In a simultaneous analysis of $N = 5525$ air, nitrogen and oxygen broadening coefficients an average accuracy is 9.2%. The parameters of the analytical model $\gamma(sur)$ may be recommended in the γ calculations of H_2O lines with rotational quantum numbers $J \leq 20$, $K_a \leq 15$ for any vibrational band from the mentioned spectral range

Keywords: water vapor, Air, N_2,O_2 and CO_2 broadening coefficients.

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Introduction

Water vapor plays a key role in attenuating solar radiation in the earth atmosphere. Knowledge of the broadening coefficients of water vapor lines by atmospheric gases is necessary for modeling atmospheric radiation processes, determining the gas concentration or temperature.

At present there is an extensive literature on experimental studies of the broadening and shift of H_2O lines by air, nitrogen, oxygen, and carbon dioxide [1–33]. These studies cover the range from 0.7 to 26000 cm^{-1}. Despite the fact, that a lot of experimental data on the broadening coefficients γ have been obtained, the need for their knowledge is much broader, so there is a need for their numerical calculation. To perform numerical calculations it is necessary to know the intermolecular interaction potentials, vibrational-rotational (VR) wave functions, as well as transition frequencies in the H_2O [34,35] molecule.

Such calculations are easy to perform for individual spectral ranges, in which the vibrational states of the molecule are combined into a separate group (polyad) of states, for which the VR wave functions and transition frequencies are calculated [36].

Approximately above 10 000 cm^{-1} such „polyad“ approach does not work, and certain approximations should be made, in order to carry out the corresponding calculations.

In this paper to calculate γ coefficients in the case of broadening of the H_2O lines by air, nitrogen, oxygen, and carbon dioxide, it is proposed to use the $\gamma(sur)$ analytical model, which was previously applied to analytical representation of γ coefficients in the case of self-broadening [37], broadening by air [14,15] and by monatomic gases [38].

The analytical model $\gamma(sur)$ depends on fitting parameters, which determine the vibrational and rotational dependence of γ coefficients. After determining these parameters from an array of experimental data (free from random errors), the $\gamma(sur)$ model can be used to calculate γ of those lines, which broadening coefficients are unknown.

Analytical model and principle of experimental data selection

To analyze the available experimental data on the broadening coefficients, we used the analytical model

$$\gamma(sur) = x_1 + x_2\Big\{1/\cosh[x_3(K_i - x_4)] + 1/\cosh[x_3(K_f - x_4)]\Big\}, \tag{1}$$

where sur denotes a surface, quantity

$$x_2 = (x_{20} + x_{26}|K_{ai} - K_{af}|)f_1(v)/\cosh\big[\big(x_{21}(J_i + J_f) + x_{22}(K_{ci} + K_{cf}) + x_{23}(K_{ci} + K_{cf})^2 + x_{24}(J_i + J_f)(K_{ci} + K_{cf}) + x_{25}(J_i + J_f)^2\big)f_2(v)\big] \tag{2}$$

is a function of vibrational (v_1, v_2, v_3) and rotational J_i, K_{ai}, K_{ci} and J_f, K_{af}, K_{cf} quantum numbers of the molecule H_2O for initial $(i) = (0, 0, 0)$ and final $(f) = (v_1, v_2, v_3)$ vibrational states in the transition $(0, 0, 0)[J_iK_{ai}K_{ci}] \rightarrow (v_1, v_2, v_3)[J_fK_{af}K_{cf}]$. For $k = 1, 3, 4$

$$x_k = x_{k0} + x_{k1}(J_i + J_f). \tag{3}$$

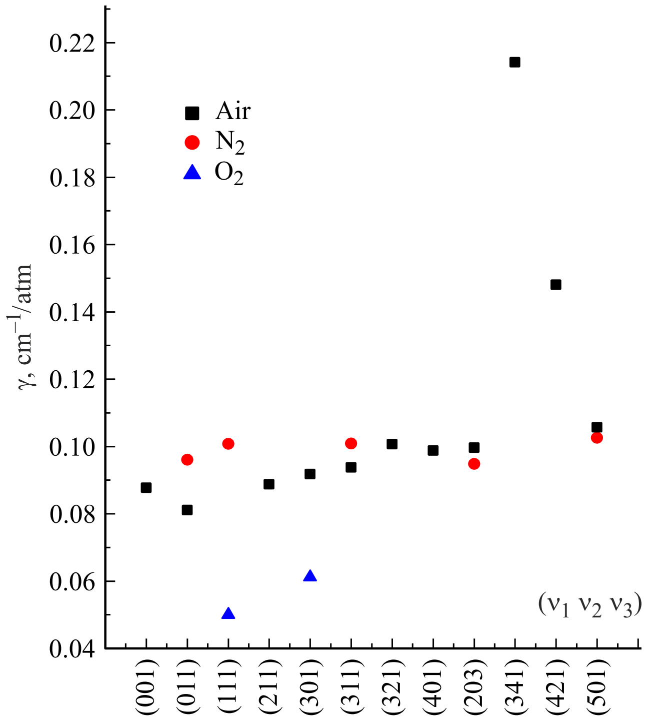

Figure 1. Vibrational dependence of the broadening coefficient γ of the water vapor line $[4\,0\,4] \leftarrow [5\,0\,5]$ in case of its broadening by air, nitrogen and oxygen. For (001), (011) and (211) the data on broadening by air are taken from [7,2] and [9] respectively, the remaining data — from [13]; for line broadening with nitrogen the data for (111) are taken from [21], the data for (221), (311), (203) — from [12], for (501) — from [22]; or line broadening by oxygen the data for (111) and (301) are taken from [24] and [6] respectively.

Functions

$$f_s(v) = 1. + t_{s1}v_1 + t_{s2}v_2 + t_{s3}v_3 \qquad (4)$$

$(s = 1, 2)$ determine vibrational dependence $\gamma(sur)$. Justification of the function (1) is given in [34,35] Parameters of the model $\gamma(sur)$ (1)–(4) are determined by fitting the expressions (1)–(4) to optimal sets of experimental data free from erroneous values. General information about the experimental data used in this work is given in Table 1.

The search for erroneous values in the experimental data $\gamma(\text{exp})$ was carried out in two interrelated ways.

In the first method, the dependence of the coefficients $\gamma(\text{exp})$ measured for the same transitions $[J_iK_{ai}K_{ci}] \rightarrow [J_fK_{af}K_{cf}]$, but for different vibrational bands $(0, 0, 0) \rightarrow (v_1, v_2, v_3)$ was analyzed. Fig. 1 shows the dependence $\gamma(\text{exp})$ on the vibrational states (v_1, v_2, v_3) for one line, and Fig. 2 — ratio R of the experimental broadening coefficients for 9 lines of the H_2O molecule obtained in [17] and [1,23] for the bands ν_1 and ν_2 respectively, in the case of line broadening by oxygen and nitrogen.

In the case of air broadening (Fig. 1), the data relating to the upper vibrational states (3, 4, 1) and (4, 2, 1) should be recognized as erroneous. These data significantly (for the band $(0, 0, 0) \rightarrow (3, 4, 1)$ are more than two times) higher, than the data obtained for other vibrational bands. There are no theoretical justifications for such an anomalously large coefficient γ for this transition in the bands $(0, 0, 0) \rightarrow (3, 4, 1)$ and $(0, 0, 0) \rightarrow (4, 2, 1)$.

The ratios R of the broadening coefficients for the transitions from Fig. 2 should be grouped around the straight line $R \approx 1.0$, but for the experimental data from [17] and [1,23] R changes from 0.9 to 3.4. The data from [17] and [1,23] are not compatible and cannot be described by a single analytic function.

Among the experimental data, there are the data, which refer to only one line. In this case, the broadening coefficient $\gamma(\text{exp})$ for this line is considered erroneous, if its addition to the common data array increases the average accuracy of restoring all data using the analytical model to $\chi_{\text{av.cr}}$. The accuracy of recovery of the coefficient γ for one line using the analytical model $\gamma(sur)$ (1)–(4) was controlled using the value

$$\chi = 100\%|1.0 - \gamma(\text{cal})/\gamma(\text{exp})|, \qquad (5)$$

and for a set of lines (related to one band or one frequency range) using the value

$$\chi_{\text{av}} = 100\% \sum_{i=1}^{N} |1 - \gamma_i(\text{cal})/\gamma_i(\text{exp})|/N. \qquad (6)$$

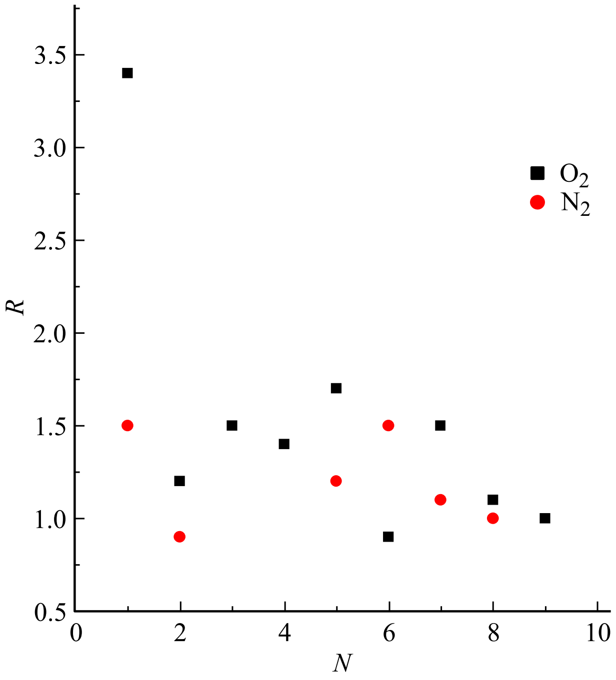

Figure 2. The ratio R of the experimental broadening coefficients for 9 lines of the H_2O molecule obtained in [17] and [1,23] for the bands ν_1 and ν_2 respectively, in case of line broadening by oxygen and nitrogen. The lines are numbered according to the Table 2 of [17].

Table 1. Experimental data on the coefficients of H_2O molecule line broadening by air, nitrogen, oxygen, and carbon dioxide used in this study*

Spectral area,	Air				Nitrogen				Oxygen				Carbon dioxide			
cm^{-1}	N_{vib}	N		χ_{av}	N_{vib}	N		χ_{av}	N_{vib}	N		χ_{av}	N_{vib}	N		χ_{av}
380-600	1	37	[4]	26.8	1	37	[4]	24.0	1	37	[4]	15.2				
600-2271	1	122	[1]	17.8	2	420	[1]	15.8								
1316-1327					1	3	[16]^a	42.0	1	3	[16]	7.6				
1212-2137									1	378	[23]	8.5	1	257	[25]	6.7
1387-1943													1	105	[26]	6.6
1630-2235	1	265	[3]	11.5												
3055-3459	1	4	[2]	5.7	1	9	[17]^a	24.2	1	9	[17]^a	20.1				
3178-4106													3	108	[26]	7.6
3450-4000	1	83	[7]	5.8									3	31	[27]	10.8
4524-5964	3	260	[2]	9.0												
6530-7718	4	291	[2]	6.1												
5300-6700	7	211	[14]	9.6												
7182-7186					1	4	[18]	4.9	1	4	[18]	12.3	2	11	[28]	7.5
7110-7190					2	8	[19]	4.1					2	8	[29]	11.3
7520-8586	11	319	[15]	7.3												
8650-9020	4	123	[20,21]	5.8	4	128	[20,24]	5.0								
10100-10800													3	168	[30]	6.6
12014-12150	1	14	[9]	9.2												
13600-13950	4	113	[6]	5.1	3	77	[6]	4.6	3	116	[6]	4.9				
13517-19847	15	216	[12]	5.3												
1950-2000					3	88	[22]	6.3								
13000-26000	60	3868	[13]	5.7												
Total	109	5803			18	769			12	675			15	688		
N_{opt}		4110				757				658				688		
χ_{av}, %	7.2				11.6				7.6				7.1			
Max(J_i, K_{ai})	(17,8)				(17,10)				(14,8)				(13,6)			

Note. *N_{vib} — number of vibrational bands from the specified range, N — number of experimental data, N_{opt} — number of experimental data included into the final analysis, from which the parameters of the analytical model (1)–(4) were determined; χ_{av} — average accuracy of experimental data recovery (in %), formula (6), *a* — removed from final fit; Max(J_i, K_{ai}) — maximum values of rotational quantum numbers J_i and K_{ai} for the lower state involved in the transition.

As in [14,15], the value $\chi_{av.cr.} = 10\%$ was chosen in this study. (This value does not apply to the data for the lines from the rotational band and ν_2 band, which are discussed below.) This value of $\chi_{av.cr.}$ is based on the following circumstance. In many experimental works, the declared error in determining the coefficients γ is several percent. However, a direct comparison of the experimental data given in the literature for the same lines shows, that the data can differ by 10–15% [39] in the case of air, nitrogen, or oxygen broadening (in the case self-broadening of water vapor lines, the difference can reach 20%). Over the time the experimental data for γ are updated, and this update can lead to a difference in the data by more than 10% (you can compare the data on the oxygen broadening from [20] and [24], microwave data [31]).

An option is possible, when the experimental data obtained for the same vibrational band, but for different rotational lines (they are given in various articles), are well restored by $\gamma(sur)$ model, but the data combined into one array are restored worse. This indicates poor compatibility of these data.

And, finally, in [15] $N = 1386$ experimental data on line broadening of 17 H_2O vibrational bands from the range 380–14000 cm^{-1} are restored by air using the model $\gamma(sur)$ (1)–(4) with an accuracy of $\chi_{av} = 9.3\%$. And only the data from the overlying range 13600–26000 cm^{-1} were included into the final (optimal) dataset, which did not increase $\chi_{av.cr.}$ above 10%.

In this study the same principle of selection of experimental data was used to obtain the parameters of the $\gamma(sur)$ (1)–(4) model.

The broadening coefficients $\gamma(\exp)$ for the lines from the rotational band and from the band ν_2 are restored from the analytical model worse than for the other strips, with $\chi_{av} \sim 19\%$ in case of expansion with air [14,15].

This may be due to the effect of narrowing the lines with high values of rotational quantum numbers, which is not taken into account by the $\gamma(sur)$ (1)−(4) model, or with the inconsistency of the data obtained for these bands. Therefore, for the bands under consideration all experimental data available in the literature were taken into account.

Results of the experimental data analysis

Air broadening. The main results were obtained in [14,15] and are given in columns 2−5 of the Table 1 for completeness. The model parameters are given in the second column of Table 2. According to the Table 1 the values of $\gamma(\exp)$ for 109 vibrational bands were analyzed, 1693 data were found to be erroneous. All of them belong to the range $13000-26000\,\mathrm{cm}^{-1}$. The average data recovery accuracy is $\chi_{\mathrm{av}} = 7.2\%$. The data restoration from the rotational band and the ν_2 band is the worst. For the rotational band the data from [1,4] are used, and, as noted in [14], these data are poorly consistent. For the band ν_2 the effect of line narrowing for high rotational quantum numbers ($J > 12$) may take place. The best accuracy with $\chi_{\mathrm{av}} = 5.1\%$ is achieved for the lines of four vibrational bands from the range $13600-13950\,\mathrm{cm}^{-1}$ studied in [6].

Nitrogen broadening. The data on nitrogen broadening belong to 18 vibrational bands from the range $380-13950\,\mathrm{cm}^{-1}$. The main difference from the data on air broadening is connected with poorly determined oscillatory dependence of the γ coefficients. This can been seen in the Fig. 1. The parameters t in the formula (4) from the model (1)−(4) are statistically poorly determined parameters, so at the final stage they were fixed by zero. The average data recovery accuracy is $\chi_{\mathrm{av}} = 11.6\%$. As in the case of air broadening, data restoration from [1,4] is the worst for the rotational band, for other bands the recovery accuracy is much better.

Oxygen broadening. Three spectral ranges, which include the bands ν_2 [23] (range $1212-2137\,\mathrm{cm}^{-1}$), $\nu_1+\nu_2+\nu_3$, $2\nu_1+\nu_2$ [20,24] (range $8650-9020\,\mathrm{cm}^{-1}$) and $2\nu_1+2\nu_2$, $2\nu_1+2\nu_2+\nu_3$, $3\nu_1+\nu_1$ [6] (range $13600-13950\,\mathrm{cm}^{-1}$) were the most fully experimentally studied. Unlike the air and nitrogen broadening, a significant increase in the broadening coefficients is observed when passing from the second to the third range, this is shown in Fig. 1 for the transition $[4\,0\,4] \leftarrow [5\,0\,5]$ (for the bands $\nu_1+\nu_2+\nu_3$ and $3\nu_1+\nu_1$) and in Fig. 3 for the transition $[4\,2\,3] \leftarrow [3\,1\,2]$ (for the bands ν_2, $2\nu_1+\nu_2$ and $2\nu_1+2\nu_2$).

Such a change in the coefficients γ leads to a large value of the parameter t_{21} from the 4th column of the Table 2 (approximately 4 times greater, than for the case of air broadening).

Coefficient ratio analysis $\gamma(v_1v_2v_3)/\gamma(v_1'v_2'v_3')$ for transitions with the same set of rotational quantum numbers, but for different vibrational bands, shows, that the ratio $\langle\gamma(221)/\gamma(111)\rangle = 1.13$, averaged over 21 transitions, averaged over 8 transitions $\langle\gamma(202)/\gamma(010)\rangle = 1.24$, and averaged over 8 transitions $\langle\gamma(210)/\gamma(010)\rangle = 1.0$. From this we can conclude, that the experimental data from the second range [24] are underestimated in relation to the experimental data from the first and third ranges studied in [23] and [6] respectively. The vibrational dependence of the broadening coefficients γ is not a linear function of the vibrational quantum numbers, which is clearly seen from Fig. 3.

The average accuracy of the experimental data recovery is 7.6%. For the data from [17] $\chi_{\mathrm{av}} = 20.1\%$, these data are inconsistent with the rest of the experimental data and were not taken into account at the final stage of determining the parameters of the $\gamma(sur)$ model.

Carbon dioxide broadening. Experimental data on the broadening of the H_2O lines were obtained for the range $1280-10800\,\mathrm{cm}^{-1}$ and refer to 15 vibrational bands.

The band ν_2 in [25,26] has been studied most completely. A comparison of 98 experimental broadening coefficients for the same transitions from this band shows, that the ratio $R = \gamma[26]/\gamma[25]$ varies from 0.91 to 1.15, averaged over all 98 transitions $R_{\mathrm{av}} = 0.98$. Model parameters (1)−(4) are given in the last column of the Table 2. Average recovery accuracy of experimental data $\chi_{\mathrm{av}} = 7.1\%$. The main difference in the parameters obtained from the parameters given in columns 2−4 is due to the parameter $x_{10} \neq 0$. The parameter x_{10} is statistically well defined. It points to the asymptotic (for large values of rotational quantum numbers) behavior of the calculated broadening coefficients. For large $J \to \infty$ the calculated $\gamma \to 0$ in the case of line broadening by air, nitrogen, or oxygen, and $\gamma \to\approx 0.04\,\mathrm{cm}^{-1}/\mathrm{atm}$ in line broadening by carbon dioxide.

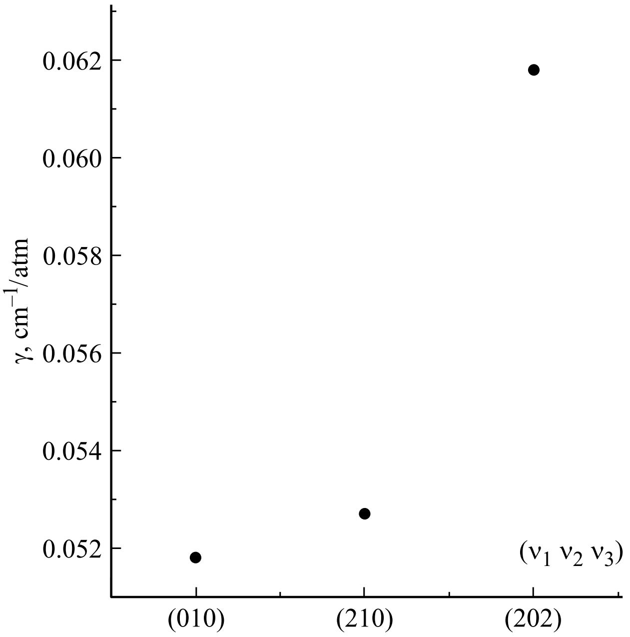

Figure 3. Vibrational dependence of the broadening coefficient γ of the water vapor line $[4\,2\,3] \leftarrow [3\,1\,2]$ in the case of oxygen broadening of the line. For (010), (210) and (202) the data are taken from [23,24] and [6] respectively.

Table 2. Parameters of the $\gamma(sur)$ analytical model found by fitting expressions (1)–(4) to the measured ($T = 296$ K) water vapor line broadening coefficients in the case of air, nitrogen, oxygen and carbon dioxide broadening (for data and spectral ranges from Table 1), temperature indicators and calculation statistics*

Parameter	Air	Nitrogen	Oxygen	Carbon dioxide
x_{10}	0.0	0.0	0.0	$0.4200(1200) \cdot 10^{-1}$
x_{20}	$0.4892(25) \cdot 10^{-1}$	$0.5436(64) \cdot 10^{-1}$	$0.2814(28) \cdot 10^{-1}$	$0.7805(125) \cdot 10^{-1}$
x_{21}	$0.2972(367) \cdot 10^{-1}$	$0.6522(545) \cdot 10^{-1}$	$0.5573(370) \cdot 10^{-1}$	$0.6505(599) \cdot 10^{-1}$
x_{22}	$-0.9190(464) \cdot 10^{-1}$	$-0.1211(90)$	$-0.1175(62)$	$-0.2129(66)$
x_{23}	$-0.5114(404) \cdot 10^{-2}$	$-0.1232(269) \cdot 10^{-2}$	$-0.1721(227) \cdot 10^{-2}$	0.0
x_{24}	$0.3692(361) \cdot 10^{-2}$	0.0	0.0	0.0
x_{25}	0.0	0.0	0.0	0.0
x_{26}	$0.1349(75) \cdot 10^{-2}$	$0.2332(352) \cdot 10^{-2}$	$0.1615(176) \cdot 10^{-2}$	$0.7480(810) \cdot 10^{-2}$
x_{30}	0.2387 (36)	0.2098(60)	0.2674(34)	0. 6238 (15)
x_{31}	$-0.1697(225) \cdot 10^{-2}$	0.0	0.0	$-0.1738(133) \cdot 10^{-1}$
t_{11}	$0.2560(115) \cdot 10^{-1}$	0.0	0.1006(47)	$0.5545(650) \cdot 10^{-1}$
t_{12}	0.0	0.0	0.0	0.0
t_{13}	$0.2002(169) \cdot 10^{-1}$	0.0	0.0	$0.6734(1376) \cdot 10^{-1}$
t_{21}	$-0.2767(340) \cdot 10^{-1}$	0.0	0.0	0.0
t_{22}	$0.1638(392) \cdot 10^{-1}$	0.0	0.0	0.0
t_{23}	$-0.4953(506) \cdot 10^{-1}$	0.0	0.0	0.0
n_2	0.702(21)			0.922(53)
n_3	0.257(58)			
χ_{av}, %	7.2 ($N = 4110$)	11.6 ($N = 757$)	7.6 ($N = 658$)	7.1 ($N = 688$)
$0 < \chi \le 10$	$N = 3207$ (78.0%)	$N = 488$ (64.5%)	$N = 490$ (74.5%)	$N = 512$ (74.4%)
$10 < \chi \le 20$	$N = 693$ (16.9%)	$N = 148$ (19.6%)	$N = 125$ (19.0%)	$N = 153$ (22.2.%)
$20 < \chi \le 50$	$N = 189$ (4.6%)	$N = 101$ (13.3%)	$N = 43$ (6.5%)	$N = 23$ (3.4%)
$\chi > 50$	$N = 21$ (0.5%)	$N = 20$ (2.6%)	$N = 0$ (0.0%)	$N = 0$ (0.0%)

Note. * Parameters x_{10}, x_{20} and x_{26} are defined in cm^{-1}/atm, other parameters are dimensionless; values $x_4 = 0$ in formula (1). The expressions $0 < \chi \le 10$ (from the first column), $N = 3207$ (78.0%) (from the second column) mean, that for $N = 3207$ lines (which is 78.0% of all $N = 4110$ lines) the value of χ varies from 0.0 to 10%.

Temperature dependence $\gamma(sur)$

To determine the temperature dependence $\gamma(sur)$, we used the literature (experimental and calculated) data on the temperature index n from the equation

$$\gamma(T) = \gamma(T_0)\left(\frac{T_0}{T}\right)^n, \tag{7}$$

where $T_0 = 296$ K.

For the case of air broadening, the indices n were taken from [3,6], for the case of carbon dioxide broadening – from [19,27], for the case of nitrogen and oxygen broadening the data for n is small, and the temperature dependence of $\gamma(sur)$ was not determined.

With indicators n using formula (7) $\gamma(T)$ for $T = 250$, 350, 380 and 400 K were calculated. Further to the calculated $\gamma(T)$ the function $\gamma(sur)$ (1)–(4) was fitted, containing in the values x_1, x_2 and x_3 taken as

$$x_k(T) = x_k(T_0)\left(\frac{T_0}{T}\right)^{n_k}, \tag{8}$$

variable n_k ($k = 1, 2, 3$)), which were determined by fitting. Other parameters $\gamma(sur)$ (1)–(4) were fixed to the values given in the Table 2. The non-zero n_k found in this way are listed in the Table 2

Joint analysis of broadening coefficients caused by air, nitrogen and oxygen pressure

Semiclassical methods for calculating the broadening coefficients γ use the intermolecular potential of the interaction „H_2O–perturbing molecule". In the case of broadening of the H_2O lines by diatomic N_2 and O_2 molecules, the potential is determined by the electrostatic and polarization interactions. In the case of broadening by air the coefficient γ is calculated by the formula

$$\gamma_{\text{air}} = 0.79\gamma_{\text{N2}} + 0.21\gamma_{\text{O2}}, \tag{9}$$

where γ_{N2} and γ_{O2} are the coefficients of nitrogen and oxygen broadening of the lines . In the present study we have verified the assumption, that the broadening of the H_2O lines by N_2 and O_2 molecules (and consequently by air) is determined by one dominant contribution to the interaction potential, which for N_2 and O_2 differs only in magnitude. This assumption was verified using formulas (1)–(4) for $\gamma(sur)$, which were used for the joint analysis of all data on the broadening coefficients of the lines H_2O by air pressure, nitrogen and oxygen. The function x_2

Table 3. Parameters of analytical model $\gamma(sur)$ found by fitting expressions (1), (3), (4), (10) to $N = 5525$ measured ($T = 296\,\mathrm{K}$) broadening coefficients of water vapor lines in case of broadening by air ($N = 4110$), nitrogen ($N = 757$) and oxygen ($N = 658$) simultaneously.

x_{20}	$0.4736(23) \cdot 10^{-1}$	t_{11}	$0.2634(109) \cdot 10^{-1}$
x_{21}	$0.6052(142) \cdot 10^{-1}$	t_{12}	0.0
x_{22}	$-0.1145(237) \cdot 10^{-1}$	t_{13}	$0.2775(176) \cdot 10^{-1}$
x_{23}	$-0.1301(80) \cdot 10^{-2}$	$m(N_2)$	$0.8935(448) \cdot 10^{-1}$
x_{24}	0.0	$m(O_2)$	$-0.4307(42)$
x_{25}	0.0	χ_{av}	9.2%
x_{26}	$0.1678(82) \cdot 10^{-2}$	χ_{av} (Air)	7.7%
x_{30}	0.2030(15)	$\chi_{av}(N_2)$	11.8%
x_{31}	0.0	χ_{av} (O_2)	15.1%

Note. * Parameters x_{20} and x_{26} are defined in cm^{-1}/atm, other parameters are dimensionless; values $x_4 = 0$ in the formula (1).

was chosen in the form

$$x_2 = (x_{20} + x_{26}|K_{ai} - K_{af}|) f_1(v) \big(1. + m(N_2) + m(O_2)\big) /$$

$$\cosh\big(x_{21}(J_i + J_f) + x_{22}(K_{ci} + K_{cf}) + x_{23}(K_{ci} + K_{cf})^2$$

$$+ x_{24}(J_i + J_f)(K_{ci} + K_{cf}) + x_{25}(J_i + J_f)^2\big), \tag{10}$$

in which the parameters $m(N_2)$ and $m(O_2)$ were additional variable parameters and differed in the total data set from the data for N_2 and O_2. All other parameters in (1), (3), (4) and (10) are common for the broadening gases under consideration.

Table 3 shows the parameters found from the simultaneous fitting of expressions (1), (3), (4), (10) to $N = 5525$ line coefficients of broadening H_2O lines by air ($N = 4110$), nitrogen ($N = 757$) and oxygen ($N = 658$) pressure. For the value χ_{av} (6), which determines the quality of recovery of all experimental data, the value $\chi_{av} = 9.2\%$ was obtained, for individual broadening gases the values $\chi_{av}(\mathrm{Air}) = 7.7\%$, $\chi_{av}(N_2) = 11.8\%$ and $\chi_{av}(O_2) = 15.1\%$ were obtained.

Comparisons $\chi_{av}(\mathrm{Air})$, $\chi_{av}(N_2)$ and $\chi_{av}(O_2)$ obtained in the joint analysis of experimental data, with similar values of χ_{av} from Table 2 obtained in a separate analysis of these data shows, that $\chi_{av}(\mathrm{Air})$ and $\chi_{av}(N_2)$ almost coincide, and $\chi_{av}(O_2)$ from the joint analysis is almost twice as large as in the separate analysis. This means, that the main contributions to the interaction potentials „H_2O-N_2" and H_2 $O-O_2$", which define line broadening, are different.

From the values of the parameters $m(N_2)$ and $m(O_2)$ it can be determined, that $\gamma(N_2)/\gamma(\mathrm{Air}) = 1.089 \pm 0.004$ and $\gamma(O_2)/\gamma(\mathrm{Air}) = 0.569 \pm 0.004$. In this case the first ratio is quite accurate, the data on air and nitrogen broadening can be analyzed along with the use of one analytical model, the accuracy is not lost. The second ratio is approximate, the oxygen broadening data can be analyzed along with the air and nitrogen broadening data, but the accuracy of the recovery of these data will be worse, than in a separate analysis.

Extrapolation to a low-lying range

Model parameters $\gamma(sur)$ from the Tables 3, 4, obtained for the range $380-26000\,\mathrm{cm}^{-1}$, were tested in calculations of line broadening coefficients from the range below 10000 GHz ($0.7-30.3\,\mathrm{cm}^{-1}$). Table 4 compares the experimental values and calculated according to the model $\gamma(sur)$ values of the coefficients γ for several transitions with known experimental values γ. In the case of line broadening by air or nitrogen for the considered transitions $\chi < 10\%$, in the case of line broadening by oxygen and carbon dioxide $\chi < 22\%$ and $\chi < 4\%$ respectively. The result can be considered quite satisfactory, given that the data were not included in the inverse problem for determining the model parameters. Determining the parameters of the model $\gamma(sur)$, which that best restore the experimental data from the range below 10000 GHz, is not the goal of this work. The calculation γ for this range is given in [8].

Comparison with the semi-classical calculation method

In [26] the most complete and high-quality calculations of the broadening coefficients γ for more than 11000 H_2O lines are presented in the case of line broadening by carbon dioxide from the range $1300-5000\,\mathrm{cm}^{-1}$. The method MCRB (modified complex Robert-Bonamy) was used, in which the parameters are from the atom-atom potential (it is part of the total interaction potential in the system „H_2O-CO_2") were selected from the condition of the best agreement between the calculations and the selected experimental data. Figure 4 compares the experimental [26] and calculated by the model $\gamma(sur)$ (with the parameters from Table 2) and in the semiclassical method [26] coefficients γ for one rotational branch from the band ν_2. It can be seen, that the calculations are in good agreement with each other, they are in good agreement with the experiment. For the known $N = 12$ experimental data from Fig. 4 $\chi_{av} = 3.5\%$ in the case of calculations using the model $\gamma(sur)$ and $\chi_{av} = 6.3\%$ with the calculations from [26]. The quality of calculations according to the model $\gamma(sur)$ and semiclassical method is also comparable in the case of other broadening gases under consideration. Calculations according to the semiclassical method are difficult for a range approximately higher, than $10\,000\,\mathrm{cm}^{-1}$, since for the H_2O molecule, the scheme for partitioning vibrational states into isolated groups does not work for this range, and certain approximations should be made to calculate the rotational frequencies of the transitions and the wave functions of the molecule. For example, all calculations are carried out without taking into account the oscillatory dependence γ.

Comparison with other analytical models

Several analytical models have been proposed in the literature for the analytical representation of the broadening

Table 4. Comparison of the experimental and calculated values of the broadening coefficients (in MHz/Torr) with the parameters from Tables 2, 3 for several H_2O lines from the range below 10000 GHz*

ν, GHz	$J_fK_{af}K_{cf} - J_iK_{ai}K_{ci}$	Air			N_2			O_2			CO_2		
		γ(exp)	γ(cal)	χ, %	γ(exp)	γ(cal)	χ, %	γ(exp)	γ(cal)	χ, %	γ(exp)	γ(cal)	χ, %
22	616–523		3.45; 3.30		4.10[c]	4.01; 3.60	2.2; 7.3	2.52[c]	1.97; 1.88	21.8; 25		4.69	
183	313–220	3.97–4.6[b]	3.70; 3.68	6.8; 7.3	4.230[b]	4.23; 4.00	0; 5.4	2.580[b]	2.15; 2.09	16/7; 19.0	6.180[b]	6.42	3.9
325	515–422	3.633[a]	3.46; 3.50	4.7; 3.7	4.011[a]	4.03; 3.81	0.5; 5.0	2.212[a]	2.00; 2.00	10.0		5.40	

Note. * *a*, *b*, *c* — The data from [32,33,40]; in the columns for γ(cal) and χ, the upper and lower rows correspond to calculations with parameters from Tables 3 and 4 respectively.

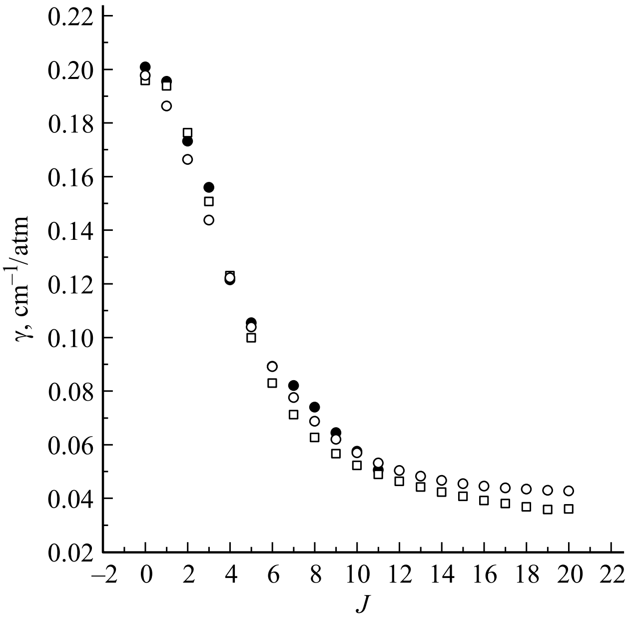

Figure 4. Experimental [26] (dark symbols) and calculated by the $\gamma(sur)$ model (symbols □) and in the semiclassical method [26] (symbols *o*) dependence of the broadening coefficient γ for the rotational branch $[J\,0\,J] \to [J+1\,1\,J+1]$ of the vibrational band ν_2 in the case of line broadening by carbon dioxide.

coefficients of water vapor lines [2,34,35,41]. In [41], as well as in this paper, a model is proposed for calculating the coefficients γ in the case of broadening of water vapor lines by air, nitrogen, oxygen, and carbon dioxide. According to [41], the broadening coefficient γ for the transition $[J\tau] \to [J'\tau']$ (τ — a general notation for rotational quantum numbers K_a, K_c can be calculated using the formula

$$\gamma_{oJ\tau - 0J'\tau'} \approx \left\{ \left[\gamma^{(n-1)}_{0J\tau - 0J\tau} + \gamma^{(n-1)}_{0J'\tau' - 0J'\tau'}\right]/2 \right\}^{1/(n-1)}, \quad (11)$$

where $\gamma_{0J\tau - 0J\tau}$ — the broadening coefficient for the fictitious (there is no such transition in the real spectrum) rotational transition $[J\tau] \to [J\tau]$, calculated in the semiclassical method, n — parameter different for different broadening gases. The calculated values of $\gamma_{0J\tau - 0J\tau}$ ($J \leq 16$, $K_a \leq 10$) and n are given in the corresponding tables from [41].

Table 5 compares the calculations of coefficients γ using the model $\gamma(sur)$ (1)–(4) and (11) for 9 lines from the band ν_1. The experimental data [17] for these lines were removed from the final fit per model $\gamma(sur)$, since they give a large deviation of the calculated coefficients from the experimental ones.

For the line $[5\ 4\ 1] \leftarrow [6\ 5\ 2]$ in case of nitrogen broadening the deviations of the calculated with $\gamma(sur)$ and with the model (11) γ values from the experimental value is 28.5 and 40.0% respectively; in case of line broadening by oxygen these deviations reach 62.7 and 58.1%. In this example, calculations with $\gamma(sur)$ correlate with calculations per model (11). Meanwhile, the deviations of the calculated with γ and with the (11) model values can be large for the transitions with large $\Delta\tau = |\tau - \tau'| \geq 3$. For example, for transitions from $\Delta\tau = 5$, the values γ may differ by several times.

Comparison with data base HITRAN

The experimental data in the HITRAN database [42] are much larger, than those used in this work to determine the parameters of the $\gamma(sur)$ model. Comparison of calculations by the $\gamma(sur)$ (1)–(4) model with data from the base [42] was carried out for a narrow spectral range 13521.0–13575.0 cm^{-1}, and broadening of lines by air is considered. The spectral ranges below 12000 cm^{-1} have been studied in the literature in more detail, than the ranges above 13000.0 cm^{-1}. Experimental data in [42] for this range are taken from [13]. In addition in [42] almost every line contains the values γ obtained either as a result of polynomial approximation of data from [43], or as a result of oscillatory approximation of data from low-lying ranges [44]. The comparison of the coefficients γ calculated according to $\gamma(sur)$ (1)–(4) model with the data from [42] for 10 lines is given in Table 6 compares the

It can be seen, that there are large discrepancies (more than 100%) between the $\gamma(sur)$ — calculations and their data [42]. Large deviations from the experimental data from [13] given in [42] for many lines are explained, according to [14,15], by erroneous values of these data. In the general case, there is uncertainty in the values of the γ coefficients for many lines from the range above 13000.0 cm^{-1}, and these lines require additional experimental study.

Table 5. Experimental [17] and calculated (in MHz/Torr) by various models the broadening coefficients of a number of H_2O lines from the ν_1 band in the case of their broadening with nitrogen and oxygen, $T = 296\,\mathrm{K}$

$J_fK_{af}K_{cf}$	$J_iK_{ai}K_{ci}$	N_2			O_2		
		Exp. [17]	$\gamma(sur)$	Cal. [41]	Exp. [17]	$\gamma(sur)$	Cal. [41]
5 4 1	6 5 2	3.90	2.79	2.3	3.75	1.40	1.57
5 3 3	6 4 2	2.99	3.33	3.1	1.72	1.78	1.93
4 4 0	5 5 1	2.97	2.74	2.17	1.72	1.35	1.52
4 4 1	5 5 0	2.68	2.74	2.17	1.53	1.35	1.53
5 3 2	6 4 3	4.18	3.41	2.9	2.57	1.78	1.81
11 0 11	12 1 12	1.0	1.2	0.73	0.45	0.49	0.43
11 1 11	12 0 12	0.7	1.2	0.73	0.55	0.49	0.43
8 2 7	9 1 8	2.1	2.7	1.56	1.10	1.32	0.75
5 2 3	6 3 4	3.5	3.8	3.25	1.85	2.03	1.92

Table 6. Broadening coefficients γ (in $\mathrm{cm^{-1}}$/atm) for 10 water vapor lines presented in the HITRAN database [42] and calculated using the $\gamma(sur)$ model (1)–(4) in case of line broadening with air, $T = 296\,\mathrm{K}$

ν, $\mathrm{cm^{-1}}$	γ, HITRAN	$v_1v_2v_3$	$J_fK_{af}K_{cf}$	$J_iK_{ai}K_{ci}$	$\gamma(sur)$	χ, %
13521.1060	0.0237^a	4 0 0	9 3 7	10 2 8	0.061	157.5
13521.1371	0.0408^c					49.6
13528.5966	0.0454^a	2 4 0	4 3 1	3 2 2	0.078	72.0
13528.5544	0.0242^c					222.8
13528.5970	0.0813^c					3.9
13528.7151	0.0345^a	4 0 0	5 1 5	6 2 4	0.082	138.1
13528.6619	$0.077\ ^b$					6.7
13529.4432	0.0464^a	3 0 1	8 4 5	9 4 6	0.065	40.1
13529.4169	0.0398^b					63.3
13529.4164	0.0624^b					4.1
13535.4162	0.0326^a	3 0 1	4 1 4	5 3 3	0.085	162.2
13535.4117	$0.054\ ^b$					58.3
13549.3313	0.1135^a	3 2 0	4 2 3	5 1 4	0.087	22.6
13549.3230	0.0889^c					1.2
13560.9112	0.1007^a	3 2 0	4 3 2	4 4 1	0.075	24.8
13560.9230	0.0775^c					2.3
13569.2356	0.0464^a	4 0 0	9 0 9	10 1 10	0.035	23.8
13569.2519	0.0368^b					3.9
13571.0559	0.0474^a	1 7 0	9 0 9	10 1 10	0.035	25.4
13571.0371	0.0644^c					45.1
13574.3815	0.0237^a	2 2 1	9 3 7	9 3 6	0.0664	180.3
13574.3408	0.0693^c					4.1
13574.3684	0.0499^c					33.1

Note. a — experimental data from [13], b — polynomial approximation of data from [43], c — oscillatory approximation of low-lying data [44] : the value χ determines the deviation $\gamma(sur)$ of the calculations from the data presented in the HITRAN database.

Discussion

The proposed analytical model $\gamma(sur)$ (1)–(4) with parameters from Tables 2, 3 is very convenient to use for calculating the broadening coefficients of γ lines of H_2O absorption from the range $380-26000\,\mathrm{cm^{-1}}$ in case of their broadening by air, nitrogen and oxygen and from the range $1212-10800\,\mathrm{cm^{-1}}$ in case of their broadening by carbon dioxide pressure.

Calculations do not require the knowledge of intermolecular interaction potentials, wave functions and transition frequencies in H_2O. The average accuracy of the recovery of experimental data determined by the value χ_{av} (6), is 7.2, 11.6, 7.6, and 7.1% in the case of line broadening by air, nitrogen, oxygen, and carbon dioxide respectively. This accuracy is comparable to the accuracy of calculations by semiclassical methods. The largest values of χ_{av} were obtained for the rotational bands and the band ν_2. For these bands the experimental data from [4] and [1] are poorly consistent, and the line narrowing effect is also possible in these bands (for $J > 12$). For other bands, the error of recovery the experimental data is comparable to the experimental accuracy (taking into account, that the experimental data agree with each other at a level of 10–15%).

The Examples of calculating coefficients γ for one rotational branch from the band ν_2 are shown in Figs 4 and 5. In the case of broadening by oxygen, there are no corresponding experimental data in the literature. Figure 6 gives an example of calculating coefficients γ for one rotational transition, but in different vibrational bands. For the case of nitrogen and oxygen broadening, the parameters from Table 2 (line a) and Table 3 (line b) were used. The parameters t from these tables define the oscillatory dependence of the coefficients in different ways. If in Table 3 these parameters are well defined for the case of air and oxygen broadening, then in Table 4 the vibrational dependence is average for all broadening gases. The value of the broadening coefficient γ for this line in the case of broadening by carbon dioxide in the band $6\nu_1 + \nu_3$ is 20% greater, than in the band ν_3. In the literature, in calculations, the vibrational dependence γ in the case of carbon dioxide broadening is not taken into account, although it clearly manifests itself in the experimental data.

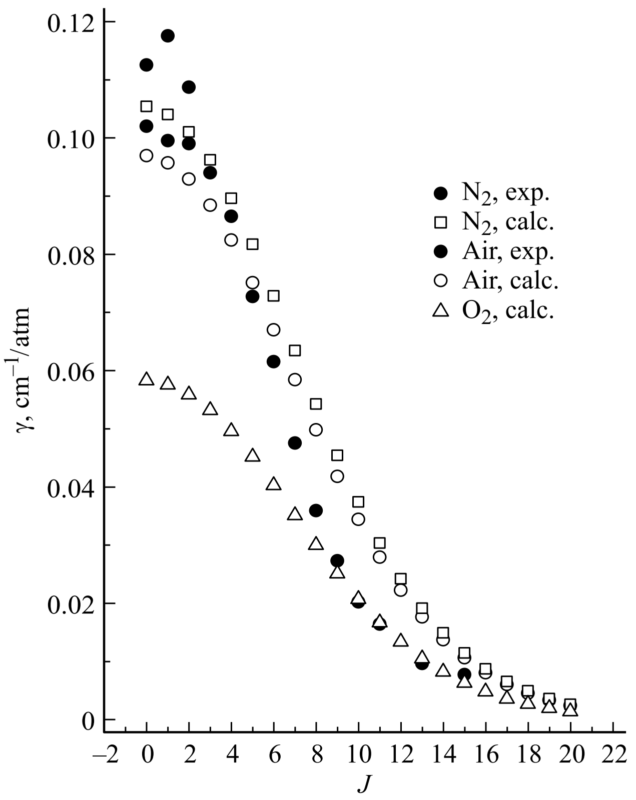

Figure 5. Experimental [1] and calculated by the $\gamma(sur)$ model dependence of the broadening coefficient γ for the rotational branch $[J\,0\,J] \to [J+1\,1\,J+1]$ of the vibrational band ν_2 in the case of line broadening by air, nitrogen, and oxygen. The parameters from the Table. 2 were used.

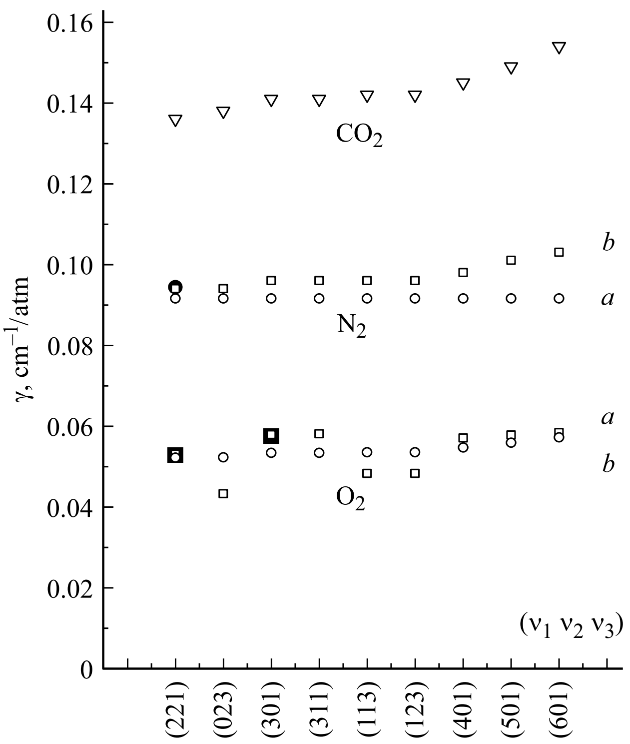

Figure 6. The experimental [6,22] (dark symbols) and calculated by the $\gamma(sur)$ model (light symbols) dependence of the broadening coefficient γ for the line $[4\,0\,4] \to [5\,0\,5]$ on vibrational quantum numbers; in the calculations *a* and *b* the parameters from the Tables 2 and 3, respectively, were used.

Conclusion

The main result of the work is contained in Tables 2, 3, which list the parameters of the $\gamma(sur)$ (1)–(4), (10) model. They contain information about 4110, 757, 658 and 688 coefficients of broadening of γ water vapor lines from the range 380–26000 cm^{-1} by air, nitrogen, oxygen and from the range 1212–10800 cm^{-1} by carbon dioxide pressure. In the experimental data from Table 1 the maximum values of the rotational quantum numbers J_i, K_{ai} for the lower VR state involved in the transition are 17 and 10, respectively. The parameters and model $\gamma(sur)$ (1)–(4), (10) can be recommended for calculating γ lines with $J_i \leq 20$, $K_{ai} \leq 15$ of any vibrational band from the indicated ranges, in the case of its broadening by the considered gases. The model extrapolation properties studied in [14] for the case of air broadening show, that the model $\gamma(sur)$ and its parameters can be successfully used for calculations of γ from the overlying ranges

In the case of oxygen broadening, it is preferable to use the parameters from Table 2, rather than from Table 3, since they more accurately recover the experimental data. Moreover, it should be noted, that in the case of oxygen broadening, a certain strong vibrational dependence is poorly confirmed by experimental data. In the case of nitrogen broadening, the vibrational dependence of γ is not statistically determined; in the case of air broadening, the vibrational dependence of γ is clearly pronounced and much weaker, than in the case of broadening with oxygen. The asymptotic behavior of the γ coefficients in the case of carbon dioxide line broadening differs from the similar behavior of γ in the case of line broadening by air, nitrogen, or oxygen. Comparison of calculations according to the $\gamma(sur)$ (1)–(4) model with the values γ given in the HITRAN database [42] in the case of air line broadening shows, that many lines lying in the range above 13000.0 cm^{-1} require additional experimental analysis.

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Conflict of interest

The author declares that he has no conflict of interest.

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