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SPECTROSCOPY OF AMBIENT MEDIUM

Self- and Air-Broadening Coefficients of $HD^{16}O$ Spectral Lines

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Abstract—We present the line broadening and self-broadening coefficients of the water isotopologue $HD^{16}O$ and study their dependence on quantum numbers up to $J = 50$ for *P*-, *Q*-, and *R*-branches. Three calculation techniques have been used: the analytical model in the case of known quantum transition identification in normal modes; the *JJ*' dependence in the case when only *J* and level symmetry are known, and the semi-empirical calculation technique for $50 \geq J > 15$.The derived regularities for the broadening coefficients of water vapor lines allow accurate calculation of $HD^{16}O$ spectra including millions of weak lines from the VTT line list (Voronin, Tennyson, and Tolchenov).

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INTRODUCTION

Atmospheric radiation transfer calculations with sufficient accuracy remain a serious difficulty in global climate simulation problems; the insufficient accuracy results, in particular, in a significant difference between the calculated and measured values of the radiation balance. Inadequate and incomplete initial spectroscopic information is one of the sources of the difference.

Knowledge of spectra of water vapor and its isotopologues, particularly, $HD^{16}O$, are required for many astrophysical applications, such as the deuterium test [1, 2], the Venus atmosphere study [3], and so on. As is known, the water vapor in the Earth's atmosphere consists of different isotopologues (relative content is given in parenthesis): $H_2{}^{16}O$ (0.997317), $H_2{}^{18}O$ (1.99983×10^{-3}), $H_2{}^{17}O$ (3.71884×10^{-4}), $HD^{16}O$ (3.10693×10^{-4}), $HD^{18}O$ (6.23003×10^{-7}), and $HD^{17}O$ (1.15853×10^{-7}) [4]. The ratio of isotopologues can differ significantly for other planets. For example, the ratio HDO/H_2O is 200–300 times higher in Venus's atmosphere than in Earth's [3].

The development and population of spectroscopic databases (DB) are urgent problems, which should be solved to determine the absorbing properties of the atmosphere. The influence of refinement of spectroscopic information on the calculation accuracy of solar radiative fluxes in the atmosphere has been analyzed in [5]. The authors [5] used different versions of the HITRAN [6, 7] and Partridge–Schwenke DBs [8]. They showed a significant dependence of a final result on input spectroscopic information.

In 1998, it was proposed that the difference between the measured and calculated data on the radiation budget in the case of clear air could be partly explained by the absence of weak lines in modern data banks [9]. Later on, it was shown that the contribution of weak water vapor lines in the solar radiation absorption by the Earth's atmosphere can reach 2 W/m^2, which is comparable with the CO_2 doubling effect [10–12]. These assessments were proved by Ptashnik in his works, e.g., [13].

It was shown in [14, 15] that the use of averaged half-width values of water vapor lines can result in a very high error in line intensities and, hence, in significant errors in atmospheric calculations. In additions, the use of the mean water line broadening coefficient (0.0964 cm^{-1}/atm in HITRAN-2000 [12] or 0.07 cm^{-1}/atm in HITRAN-2004) can result in a transmission coefficient error of up to 3% [15] at a spectral resolution of about 0.01 cm^{-1}.

The VTT line list (Voronin, Tennyson, Tolchenov) [16] is the most complete and exact; it includes $HD^{16}O$ line centers and intensities. The VTT line list has been calculated on the basis of the DVR3D discrete coordinate method [17] using the potential [18] and the dipole moment surface [19]. It is accessible freely on websites [20, 21] and includes all the theoretically probable transitions for rotational quantum numbers up to $J = 50$ (about 700000000 transitions) in a range of up to 25600 cm^{-1}. It should be noted that Partridge

Table 1. Number of lines of main H_2O isotopologues included in DBs

Data bank	H_2O isotopologues			
	$H_2{}^{16}O$	$H_2{}^{18}O$	$H_2{}^{17}O$	$HD^{16}O$
HITRAN-96	30117	6357	3744	9226
HITRAN-2000	31646	7423	3755	8493
HITRAN-2004	32372	9532	6119	9626
HITRAN-2008	37432	9754	6993	13238
Calculation [8]	289806	64734	46003	96102 [22]
BT2 [24]	505806202	–	–	–
VTT [16]	–	–	–	697454528

and Schwenke earlier obtained the line list for 100000 transitions in a range of up to 20000 cm^{-1} [8, 22]; a more extensive calculation was carried out by Tashkun [23] (up to 25000 cm^{-1}, more than 250000 transitions). Table 1 shows the number of lines of water molecule isotopologues presented in different databases.

It is evident that the VTT line list is the most complete for $HD^{16}O$.

Unfortunately, the lack of air- and self-broadening coefficients makes the use of VTT difficult. In this work, we suggest a calculation technique for air- and self-broadening coefficients of $HD^{16}O$ lines.

Let us note that the half-widths of the lines weakly depend on vibrational quantum numbers; half-widths of different bands differ by not more than several percent (see [25]). The rotational dependence of the broadening coefficients was analyzed in detail earlier based on the analysis of contribution of different types of intermolecular interactions and different scattering channels [26]. The conclusion has been drawn in the work that the rotational dependence has a more complicated character, as was supposed earlier, and its main regularities have been ascertained. This, in its turn, allows half-widths to be forecast from the rotational quantum numbers J, K_a, and K_c in the normal modes. Therefore, the rotational dependence of broadening coefficients was our principal interest.

Calculations of the broadening parameters of rovibrational lines of molecular gases within the Robert–Bonamy (RB) semiclassical theory [27], proceeded from accurate simulation of intermolecular potential and, accounting for fine details of collisions and intramolecular dynamics, require the use of quite complicated and long calculations, even for one line. The calculations for the IR and visible spectra are quite time-consuming. Hence, the calculation procedure needs simplifying while maintaining its accuracy. In addition, modern semiclassical methods are impossible to use without a complete set of rovibrational quantum numbers. In the VTT line list, 20% of lines have no quantum numbers in the normal modes conventionally used in data banks (V_1, V_2, V_3, K_a, and K_c), but only "good" quantum numbers: J, symmetry, and a level number. Therefore, we used different approaches for determining half-widths depending on the presence of a complete set of quantum numbers.

CALCULATION TECHNIQUES FOR BROADENING COEFFICIENTS

Three calculation techniques have been used: 1) the technique [28] in the case of a known quantum transition identification in normal modes; 2) the JJ' dependence [29] in the case when only J and the level symmetry are known; 3) the semiempirical calculation technique [30] for $50 \geq J > 15$.

In the first case, the analytical model [28] was used to calculate the self-broadening coefficients. This model is based on the fact that the self-broadening coefficients γ_{if} in the case of a strong dipole-dipole interaction can be calculated in the ATC approximation [31] as

$$\gamma_{if} = \frac{nv}{2\pi c} \times \pi b_0^2 \left\{ 1 + \frac{1}{b_0^4}\frac{4}{9}\left(\frac{\mu_1\mu_2}{\hbar v}\right)^2 [\Phi_{11}(J_i, \tau_i)] + (i \to f) \right\}, \tag{1}$$

where μ_1 and μ_2 are the dipole moments of interacting molecules; J and $\tau \equiv (K_a, K_c)$ are the rotational quantum numbers of an absorbing molecule; v is the relative velocity of colliding molecules; n is the density of perturbing molecules, and

$$\Phi_{11}(J_i, \tau_i) = \sum_{J_2} \rho_{J_2} \sum_{i'2'} \left| D_1(i'; i) D_1(2'; 2) \right|^2 F_1(k_0). \tag{2}$$

Here D is the rotational matrices, b_0 is the interruption parameter, ρ_{J2} are the statistical weights of the levels of a broadening molecule, $F_1(k_0)$ is the "large" resonance function for the dipole-dipole interaction, the argument of which is determined by the frequencies of virtual transitions. Eqs. (1) and (2) show that the coefficients γ_{if} are determined by combinations of the resonance functions $F_1(k_0)$, calculated for different arguments k_0. The resonance function $F_1(x)$ is shown in Fig. 1 (black circles).

The empty circles show the analytical function $F_1^{\text{mod}}(x) = a_1/\cosh[\alpha(x - x_e)]$ modeling $F_1(x)$. It is seen that the resonance function falls as $1/\cosh[\alpha x]$ at large values of the argument x, which correspond to large values of the rotational quantum numbers.

The linear combination of the functions $F_1(k_0)$ in Eq. (2) also has the form of the resonance function $F_1^{\text{mod}}(x)$, but with other parameters α and x_e, depending on the rotational quantum numbers J and τ. The representation of the linear combination of resonance functions $\Phi_{11}(J_i, \tau_i)$ (2) as the new model resonance function

$$\Phi_{11}(J_i, K_i) = \frac{a_{11}(J_i, K_i)}{\cosh[\alpha_1(J_i)(K_i - x_{e1}(J_i))]} \tag{3}$$

results in the following analytical expression for γ_{if}:

$$\gamma_{if} = x_0 + \left\{\frac{x_1(J_i, K_i)}{\cosh[\alpha_1(J_i)(K_i - x_{e1}(J_i))]} + \frac{x_1(J_f, K_f)}{\cosh[\alpha_1(J_f)(K_f - x_{e1}(J_f))]}\right\}, \tag{4}$$

where $K = K_a$;

$$x_0 = \frac{nv}{2c} b_0^2, \tag{5}$$

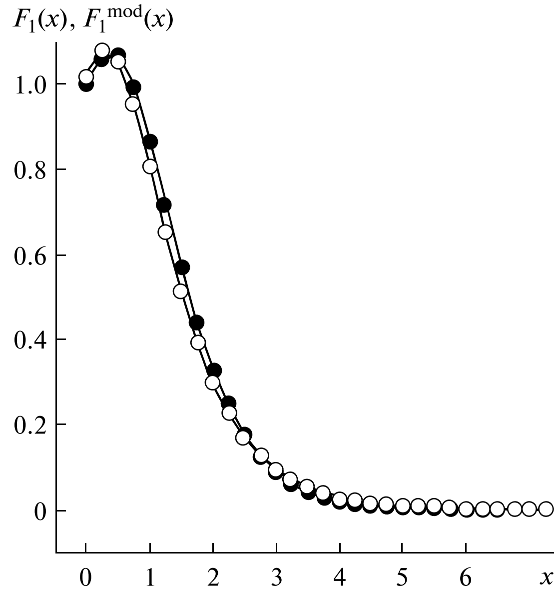

Fig. 1. Resonance $F_1(x)$ (dark circles) and analytical $F_1^{\text{mod}}(x)$ (empty circles) functions.

$$x_1(J_i, K_i) = \frac{nv}{2c}\frac{1}{b_0^2}\frac{4}{9}\left(\frac{\mu_1\mu_2}{\hbar v}\right)^2 a_{11}(J_i, K_i). \tag{6}$$

Modification of Eq. (4) results in the equation

$$\gamma_{if} = x_1 + \frac{x_2(J_i, K_i)\cosh[\alpha_0(J_i)(K_i - K_f)(K_i + K_f)]}{\cosh[\alpha_1(J_i)(K_i - x_{e1}(J_i))]\cosh[\alpha_1(J_i)(K_f - x_{e1}(J_f))]}. \tag{7}$$

Equations (4) and (7) are equivalent for use in interpolation. In this work, we have chosen Eq. (7). The self-broadening coefficients should behave like the resonance functions, i.e., decrease like $1/\cosh[\alpha(J)K]$, in the asymptotics of large rotational numbers. The following expansion was used for any function x_1, x_2, $\alpha_0 = x_5$, $\alpha_1 = x_3$, and $x_{e1} = x_4$ in Eq. (7):

$$x_k = x_{k0} + x_{k1}(J_i + J_f). \tag{8}$$

The subscript i relates to the lower state, and the subscript f, to the upper one.

The model parameters x_{k0} and x_{k1} was found using the least squares method from fitting Eq. (7) to 2738 values of the broadening coefficients γ, given in the HITRAN DB for ν_2, $\nu_2 + \nu_3$, $2\nu_2$, $2\nu_2 + 3\nu_3$, $\nu_1 + 3\nu_3$, $3\nu_1 + 3\nu_2$, $4\nu_1 + \nu_2$, $5\nu_1$, and $4\nu_3$, with the maximum values of the rotational quantum numbers $J = 17$ and $K_a = 8$. The derived functions are

$$x_1 = 0.141622, x_2 = 0.383127 - 0.812351 \times 10^{-2}(J_1 + J_2);$$

$$\alpha_1 = 0.134415 + 0.10193 \times 10^{-1}(J_1 + J_2),$$

$$x_{e1} = -1.37783 + 0.251547(J_1 + J_2),$$

$$\alpha_0 = 0.0229364.$$

The subscript 1 relates to the upper state, and the subscript 2, to the lower one.

Similar calculations have been carried out for the case of air broadening of $HD^{16}O$ lines as well.

The accuracy of air-broadening coefficient retrieval is 5.8%. Fitting to the broadening coefficients, known from the HITRAN DB, we have derived the functions

$$x_2 = 0.107718 - 0.158735 \times 10^{-2}(J_1 + J_2);$$

$$\alpha_1 = 0.159233 + 0.239003 \times 10^{-2}(J_1 + J_2),$$

$$x_{e1} = -0.587627 + 0.179593 \times 10^{-2}(J_1 + J_2);$$

$$\alpha_0 = -0.031783 + 0.662095 \times 10^{-3}(J_1 + J_2).$$

Analytical model (7) with the parameters found allows asymptotic behavior of the broadening coefficients at large values $J \sim 50$ and $K_a \sim J$ to be studied.

The described technique uses the quantum numbers J and K_a of the upper and lower states. If K_a of the upper and (or) lower states is unknown, we used the JJ' dependence, similar to that described in [29]. One

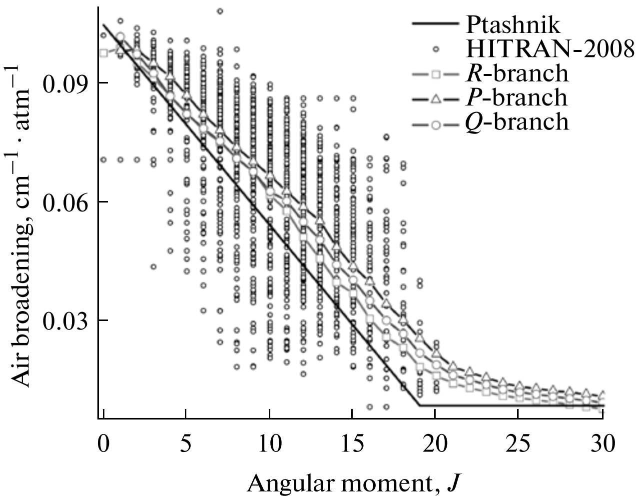

Fig. 2. Air-broadening coefficients of HD^{16}O lines from the HITRAN-2008 DB (circles) and the work [5] by Ptashnik and Shine (solid curve) versus *J*, and the *J'J''* dependencies for the *P*-, *Q*-, and *R*-branches.

may say that the *JJ'* dependence is the development of the quite popular *J* dependence, when the contour parameters are averaged for every *J* over a large data volume, e.g., HITRAN or GEISA. Thus, the data are quite roughly estimated. It was shown in [29], and is shown here, that there is a definite dependence of line broadening on the branch type (*P*, *Q*, or *R*). Its physical basis is not clear and, probably, can be a subject of an individual study. We show that this dependence exists.

A rotational dependence of the HD^{16}O broadening coefficients has been derived separately for *P*-, *Q*-, and *R*-branches (see Fig. 2 and Table 2 below). The HD^{16}O symmetry is lower than that of the main water isotopologue; hence, the symmetry division has no sense. The data for *Q*-branch actually mean the *J* dependence.

To find the dependence of the broadening coefficients at large rotational quantum numbers $J > 13$ (there are no experimental data for the corresponding lines), the calculations have been carried out within the semiempirical method developed earlier [26, 30, 32], including different corrections caused by deviations from the Anderson approximation.

Within the semiclassical impact theory, the halfwidth of the spectral line associated with the $i \to f$ transition can be represented as

$$\gamma_{if} = A(i,f) + \sum_l D^2(ii' \mid l) P_l^A(\omega_{ii'}) + \sum_l D^2(ff' \mid l) P_l^A(\omega_{ff'}) + \ldots. \qquad (9)$$

Here

$$A(i, f) = \frac{n}{c} \sum_2 \rho(2) \int_0^\infty v dv b_0^2(v, 2, i, f)$$

is the typical summand of the Anderson theory conditioned by the molecule interruption ($b_0(v, 2, i, f)$ is the interruption parameter); $\rho(2)$ is the population of buffer molecule levels. The transition strengths $D^2(ii'|l)$ and $D^2(ff'|l)$, related to the $i \to i'$ and $f \to f'$ scattering channels, depend only on the properties of the absorbing molecule and include only intramolecular effects. The terms with $l = 1$ relate to the dipole transitions, and $l = 2$ corresponds to the quadrupole transitions of the main molecule. The expansion coefficients $P_l^A(\omega_{ii'})$, known as the interaction efficiency functions, depend on the properties of absorbing and perturbing molecules. They depend on the intermolecular potential, the trajectories of colliding molecules, the structure of energy levels, and the wave functions of the perturbing molecule. These parameters can be considered as the efficiency functions for the given scattering channel. Let us introduce the correcting multiplier to this function without changing the term $D^2(ii'|l)$, which describes the dynamics of absorbing molecule:

$$P_l(\omega) = P_l^A(\omega)[l + a_1(\omega) + a_2(\omega)^2 + \ldots], \qquad (10)$$

where $P_l^A(\omega)$ is the efficiency function in the Anderson approximation. The expression in the square brackets is the correction to different effects neglected in the Anderson theory. Broadening of HD^{16}O lines was calculated with the use of the efficiency function in the following form:

$$P_l(\omega_{ff'}) = P_l^A(\omega_{ff'})[c_1/c_2 + \sqrt{j_f}]. \qquad (11)$$

Here c_1 and c_2 are the parameters found from fitting to the experimental values.

RESULTS AND DISCUSSION

Using the three above-described techniques, we match each line from the VTT line list with the self- and air-broadening and temperature dependence coefficients. The developed software for estimating the parameters of spectral line contours in such a way, calculated with the use of VTT DB, is freely accessible on the website http://www.exomol.com/.

To estimate the contribution of weak water vapor lines to the solar radiation absorption by the Earth's atmosphere, the linear dropping *J* dependence of halfwidths was used in [5] and the *J* dependence obtained through averaging over all HITRAN-2000 lines, in [12]. Figure 2 shows the air-broadening coefficients for all HD^{16}O transitions from the HITRAN-2008 DB [5] and *J'J''* dependencies for *P*-, *Q*-, and *R*-branches from this work.

Table 2. Air- and self-broadening coefficients of HD^{16}O lines (P-, R-, and Q-branches) versus J of the upper level in the range from 0 to 50

J'	Air broadening, cm^{-1}/atm			Self-broadening coefficient, cm^{-1}/atm			n_{air}	J'
	Branch							
	R	P	Q	R	P	Q		
0	0.0969	–	–	0.4550	–	–	0.78	0
1	0.0981	0.0975	0.1010	0.4663	0.4587	0.4530	0.78	1
2	0.0944	0.0977	0.0966	0.4597	0.4627	0.4605	0.78	2
3	0.0906	0.0943	0.0918	0.4466	0.4571	0.4493	0.77	3
4	0.0861	0.0909	0.0860	0.4212	0.4473	0.4258	0.73	4
5	0.0817	0.0862	0.0815	0.3996	0.4206	0.3987	0.69	5
6	0.0775	0.0814	0.0779	0.3710	0.3989	0.3740	0.64	6
7	0.0744	0.0774	0.0747	0.3501	0.3721	0.3554	0.59	7
8	0.0705	0.0731	0.0703	0.3243	0.3475	0.3333	0.53	8
9	0.0670	0.0695	0.0670	0.3006	0.3231	0.3161	0.49	9
10	0.0611	0.0660	0.0620	0.2816	0.3032	0.3019	0.45	10
11	0.0571	0.062	0.0596	0.2614	0.2935	0.2809	0.41	11
12	0.0505	0.0581	0.0543	0.2289	0.2705	0.2632	0.39	12
13	0.0451	0.0545	0.0498	0.2053	0.2504	0.2364	0.37	13
14	0.0391	0.0480	0.0436	0.1897	0.2196	0.2046	0.36	14
15	0.0363	0.0431	0.0397	0.1741	0.1887	0.1814	0.36	15
16	0.0299	0.0392	0.0345	0.1623	0.1751	0.1687	0.38	16
17	0.0253	0.0336	0.0295	0.1510	0.1625	0.1568	0.41	17
18	0.0226	0.0296	0.0261	0.1408	0.1512	0.1460	0.41	18
19	0.0178	0.0249	0.0213	0.1316	0.1410	0.1363	0.41	19
20	0.0156	0.0210	0.0183	0.1234	0.1318	0.1276	0.41	20
21	0.0136	0.0178	0.0157	0.1159	0.1235	0.1197	0.41	21
22	0.0125	0.0164	0.0145	0.1092	0.1160	0.1126	0.41	22
23	0.0115	0.0151	0.0133	0.1030	0.1093	0.1062	0.41	23
24	0.0105	0.0137	0.0121	0.0975	0.1031	0.1003	0.41	24
25	0.0100	0.0128	0.0114	0.0924	0.0976	0.0950	0.41	25
26	0.0094	0.0123	0.0109	0.0878	0.0925	0.0902	0.41	26
27	0.0089	0.0118	0.0103	0.0836	0.0879	0.0858	0.41	27
28	0.0083	0.0114	0.0098	0.0796	0.0836	0.0816	0.41	28
29	0.0077	0.0109	0.0093	0.0761	0.0797	0.0779	0.41	29
30	0.0072	0.0104	0.0088	0.0727	0.0761	0.0744	0.41	30
31	0.0065	0.0098	0.0081	0.0697	0.0728	0.0713	0.41	31
32	0.0058	0.0091	0.0075	0.0668	0.0697	0.0683	0.41	32
33	0.0052	0.0084	0.0068	0.0642	0.0668	0.0655	0.41	33
34	0.0045	0.0078	0.0061	0.0617	0.0642	0.0630	0.41	34
35	0.0038	0.0071	0.0055	0.0594	0.0617	0.0606	0.41	35
36	0.0037	0.0069	0.0053	0.0572	0.0594	0.0583	0.41	36
37	0.0036	0.0067	0.0051	0.0552	0.0572	0.0562	0.41	37
38	0.0035	0.0065	0.0050	0.0533	0.0552	0.0543	0.41	38
39	0.0034	0.0063	0.0048	0.0515	0.0533	0.0524	0.41	39
40	0.0033	0.0061	0.0047	0.0498	0.0515	0.0507	0.41	40
41	0.0032	0.0059	0.0045	0.0483	0.0498	0.0491	0.41	41
42	0.0030	0.0057	0.0043	0.0467	0.0483	0.0475	0.41	42
43	0.0029	0.0054	0.0042	0.0453	0.0468	0.0461	0.41	43
44	0.0028	0.0052	0.0040	0.0440	0.0453	0.0447	0.41	44
45	0.0027	0.0050	0.0038	0.0427	0.0440	0.0434	0.41	45
46	0.0026	0.0048	0.0037	0.0416	0.0427	0.0422	0.41	46
47	0.0025	0.0046	0.0036	0.0403	0.0416	0.0410	0.41	47
48	0.0025	0.0045	0.0035	0.0393	0.0404	0.0399	0.41	48
49	0.0024	0.0043	0.0033	0.0383	0.0393	0.0388	0.41	49
50	0.0023	0.0041	0.0032	0.0372	0.0383	0.0378	0.41	50

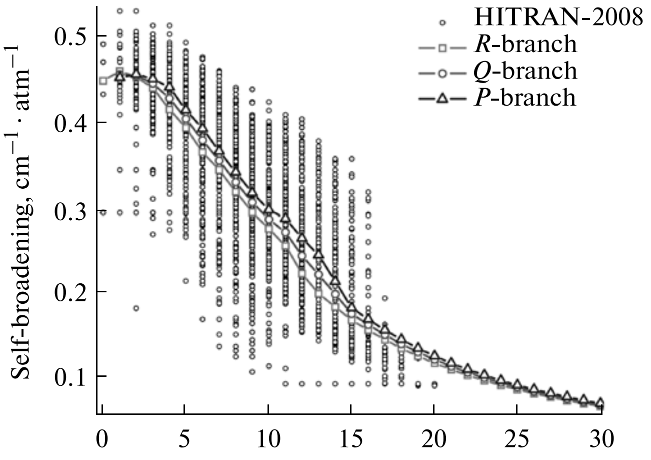

Fig. 3. Self-broadening coefficients of HD^{16}O lines from the HITRAN-2008 DB (circles) and our estimates for the *P*-, *Q*-, and *R*-branches.

For the $J'J''$ dependence, the air-broadening coefficients for large J were estimated with the use of the semiempirical technique (see Eq. (9)). Numerical $J'J''$ values are given in columns 2–4 of Table 2.

Figure 3 shows the HD^{16}O self-broadening coefficients from the HITRAN-2008 DB and our coefficients for *P*-, *Q*-, and *R*-branches. The same data are given in columns 5–7 of Table 2. The coefficients for $J > 13$ (*P*-, *Q*-, and *R*-branches) have been obtained by averaging the self-broadening coefficients for all theoretically probable transitions of a given branch from a given J, calculated by Eq. (7).

For example, $20_{0.20} \to 20_{1.19}$, $20_{2.19}$, $20_{3.17}$, $20_{3.16}$, etc.; $20_{1.20} \to 20_{1.19}$, $20_{2.19}$, ... etc. transitions and the transitions from the lower levels with another symmetry: $20_{1.19} \to 20_{0.20}$, $20_{1.20}$, ... etc. were calculated for the *Q*-branch and $J = 20$.Then all transitions were averaged, and one value for $J = 20$ of the *Q*-branch was found. Using the HITRAN DB, similar averaging procedure can be carried out only for $J < 13$ because of the lack of data for different types of transitions. There are practically no transitions from levels for which $J \sim K_a$ and $K_a \sim K_c$ for large J, but only transitions from levels for which $J \sim K_c$.

The averaged values, used in HITRAN, can be also noted in Fig. 3, e.g., 0.1 cm^{-1} for the data series from $J = 10$ to $J = 20$.

Table 2 shows the data obtained for air- and self-broadening depending on the band type and the rotational quantum number J.

The temperature dependence coefficient from Table 7 in [6] is given in the next to last column.

The air-broadening coefficients for HD^{16}O transitions from the HITRAN-2008 DB are compared with our data obtained with the use of Eq. (7) and the $J'J''$ dependence, and with data from [5] in Fig. 4.

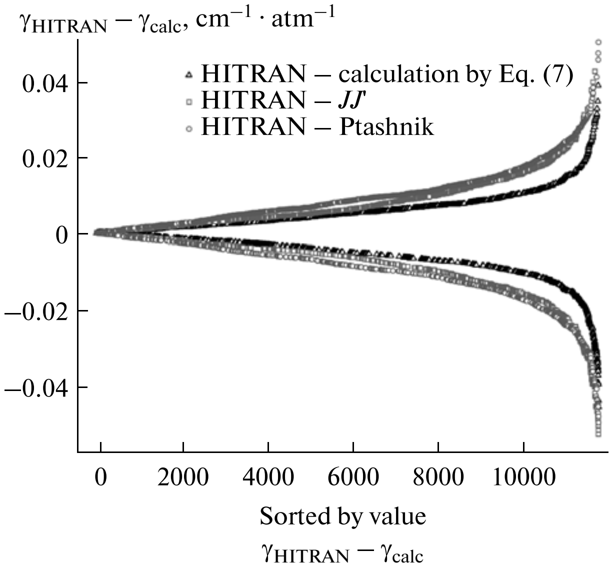

Fig. 4. Comparison of the HITRAN-2008 HD^{16}O air-broadening coefficients with those calculated using Eq. (7), the JJ' dependence, and the linear estimate [5].

For the comparison, first, all the HITRAN-2008 data with large errors in air broadening, intensities, and transition centers were removed. Thus, 11792 air-broadening coefficients remained. There are complete quantum identification sets for these transitions, which allowed us to estimate line broadening using three techniques: by Eq. (7), with the use of $J'J''$ dependence (see Table 2), and using the linear dependence from [5]. The half-width values, obtained with the use of these three techniques, were compared with the data [6]. The ascending sorted deviations (the sorting was carried out modulo) are shown in Fig. 4. As is seen, the data obtained by Eq. (7) are in the best agreement with the HITRAN-2008 data; the maximum deviations in this case do not exceed 0.04 cm^{-1}.

CONCLUSIONS

The broadening, self-broadening, and temperature dependence coefficients are obtained for all theoretically permitted HDO transitions from the VTT line list [16] in a range of up to 25000 cm^{-1} and for $J < 51$.

Thus, we can say that we obtain the parameters of line profiles with accuracy sufficient for many applications.

It is shown that the JJ' dependencies act not only for the main isotopologue H$_2$^{16}O (see [29]), but also for HDO.

Approaches to calculations of the HDO broadening and self-broadening coefficients, presented in this work, can be also applied for the Partridge–Schwenke line list [8, 22].

The VTT-HW.f90 program for calculating half-widths and self-broadening for the VTT line list is available on the websites http://www.exomol.com/ and ftp://ftp.iao.ru/pub/VTT.

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