Analytical-function correction to the Hartmann–Tran profile for more reliable representation of the Dicke-narrowed molecular spectra

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A B S T R A C T

The β-corrected Hartmann–Tran profile (HTP) constitutes an approximation of the partially correlated quadratic speed-dependent billiard-ball profile (SDBBP) easily applicable in calculations. We extend the approach originally developed for self-perturbed molecules [Wcisło et al. J. Quant. Spectrosc. Radiat. Transf. 177, 75–91 (2016)] to systems with a wide range of perturber-to-absorber mass ratios, including those relevant for atmospheric studies. This approach combines the computational simplicity of the HTP with the more physically justified rigid-sphere model for velocity-changing collisions. It is important for the analysis of high-resolution spectra influenced by the Dicke-narrowing effect. The β-corrected HTP enables high quality analytical representation of experimental spectra without incurring the high computational cost of more advanced line-shape models. This correction is directly applicable to any other line-shape model based on the hard-collision model for velocity-changing collisions.

1. Introduction

For an accurate description of spectral line shapes of isolated molecular transitions in the gas phase, it is typically required to go beyond [1,2] the Voigt profile, which ignores the influence of the speed-dependence of collisional broadening and shift [3,4] as well as velocity-changing (VC) collisions [5–8] on the line shapes. It has been shown in several publications that the choice of the VC collision model and the resulting spectral line-shape profile is of fundamental importance in the analysis of high-resolution spectra [9,10]. Following Lance et al. [2] and Pine [11], in the Hartmann–Tran profile (HTP) [12], which was recommended for high-accuracy spectroscopic applications [13] and implemented in the 2016 edition of the HITRAN database [14,15], the hard-collision (HC) model [7,8] for VC collisions is used. It assumes that the active molecule after the collision has a velocity randomly selected from the Maxwellian distribution. However, it was shown that the HC model does not satisfactorily reproduce line shapes with a prominent Dicke narrowing [5] caused by VC collisions, e.g. molecular hydrogen transitions [10]. The simplest physically justified model for the VC collisions is the rigid-sphere model (also called

the billiard ball (BB) model) [16–18], which takes into account the mass ratio of colliding molecules and models the relative importance of speed- and direction-changing collisions [10,18–20]. The rigid-sphere model is used in the billiard-ball profile [16] and the speed-dependent billiard-ball profile (SDBBP) [18]. The perturber-to-absorber mass ratio α is a crucial parameter in determining the respective influence of velocity- and speed-changing collisions on the line shapes. Moreover, it is important to emphasize that calculations of a ratio of speed- and velocity-changing collision rates as well as a collision kernel based on the rigid-sphere model are in good agreement with classical molecular dynamics simulations (CMDS) [10,19,21].

In this work, we propose a correction to the frequency of VC collisions, ν_{VC}, of the HC model adopted in the HTP, in order to achieve percent-level agreement between the corrected HTP and the SDBBP. This approach was first proposed in Ref. [15] for H_2 spectra and was called the β correction. Typically when the original HC model is used to interpret experimental data, the obtained ν_{VC} scales non-linearly with pressure, which is not physical. The reason for it is that the HC model oversimplifies the actual description of the velocity changes. The correction reduces the non-linearity of the HC-based ν_{VC} with pressure. It allows finding a single ν_{VC}/pressure coefficient in multispectrum fit analysis of experimental data [22,23], which results in fidelity of spectra representation comparable to the one of the rigid-sphere model but at

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the same time keeps the low computational cost of the Hartmann–Tran algorithm. Here, we extend this approach to other molecular systems characterized by α from 0 to 5. It should be noted that the β correction does not add any extra fitted parameter to the HTP.

The proposed correction is important considering the recent rapid developments of ultra-accurate spectroscopic measurements, where accuracy is no longer limited only by experimental imperfections but also by the use of oversimplified line-shape models. The latter contribution is currently the dominant factor limiting the improvement of the accuracy of spectroscopic data. The correction will allow increasing the accuracy of line shape modeling in various fields of optical metrology, such as Doppler-broadening thermometry [24,25].

2. Velocity-changing collisions

The velocity-changing collisions reduce the mean free path of an active molecule and lead to the Dicke narrowing [5] of Doppler broadened spectral lines. One of the simplest models describing the VC collisions is the HC model, which is the one adopted in the HTP. In the HC model the velocity after the collision is randomly chosen from the Maxwell distribution $f_m(\vec{v})$ of the active molecule velocity $\vec{v}$. The corresponding HC kernel

$$f_{HC}\left(\vec{v} \leftarrow \vec{v}'\right) = \nu_{VC} f_m(\vec{v}) \tag{1}$$

describes the rate of velocity changes from the velocity before the collision $\vec{v}'$ to the velocity after the collision $\vec{v}$. A more physically justified description of the VC collisions is given by the BB model [16–18]. The BB collision model is based on the assumption that the molecular interaction potential can be approximated by a hard-sphere wall, see e.g. Refs. [10,26]. The BB kernel is given by the following analytical formula [27]:

$$f_{BB}\left(\vec{v} \leftarrow \vec{v}'\right) = \nu_{VC} f_D \frac{3}{32\pi v_m^2} \frac{(1+\alpha)^{5/2}}{\alpha^2} \frac{1}{\sqrt{v^2 - 2vv'\cos\theta + v'^2}}$$
$$\times \exp\left(-\frac{(1-\alpha)^2}{4\alpha}\frac{v'^2}{v_m^2} - \frac{(1+\alpha)^2}{4\alpha}\frac{v^2}{v_m^2} - \frac{(1+\alpha)(1-\alpha)}{2\alpha}\frac{vv'}{v_m^2}\right)$$
$$\times \cos\theta + \frac{\alpha\sin^2\theta}{v^2 - 2vv'\cos\theta + v'^2}\frac{v^2v'^2}{v_m^2}\right), \tag{2}$$

where $\nu_{VC} = v_m^2/\left(2D^{(0)}f_D\right)$ [17,18] is the effective frequency of the VC collisions, v_m is the most probable speed of the active molecule and

$$D^{(0)} = \frac{3}{8}\sqrt{\frac{k_B T}{2\pi\mu}}\frac{1}{N\sigma^2} \tag{3}$$

is the first-order mass diffusion coefficient for rigid spheres, $f_D = D/D^{(0)}$ and D is the exact mass diffusion coefficient for the rigid spheres [17]. The notation in Eqs. (2) and (3) is as follows: $\alpha = m_p/m_a$ is the perturber-to-absorber mass ratio, $\mu = m_a m_p/(m_a + m_p)$ is the reduced mass of the collision pair, θ is the scattering angle between the velocity vectors $\vec{v}$ and $\vec{v}'$, σ is the average of the rigid-sphere diameter of the absorber and the perturber, N is the number density of the perturber, k_B is the Boltzmann constant and T is temperature. As shown in Ref. [10,26], the BB collision kernel is in a good agreement with the CMDS collision kernel, provided that σ in Eq. (3) is chosen so that the hard-sphere wall intersects the short-range repulsive part of the actual potential at the mean collision energy.

3. Correction of ν_{VC} in the HTP

In Ref. [12], an algorithm for evaluating the partially-correlated quadratic speed-dependent hard-collision profile (pCqS-DHCP) [11] with the computational time comparable to that of

the standard Voigt profile was introduced. The IUPAC Task Group [13,14] recommended to call this fast algorithm the Hartmann–Tran profile and demonstrated its utility by applying it to the analysis of water spectra. In Refs. [12,28] the HTP was applied to spectral analysis of other molecules. The way of storing the HTP parameters in the HITRAN2016 database was presented in Ref. [15] and recently extended to the double-power-law representation of the temperature dependencies of the line-shape parameters [29]. The HTP is described by the following set of parameters:

$$HTP(\Gamma_D, \Gamma_0, \Delta_0, \Gamma_2, \Delta_2, \nu_{VC}, \eta, \Delta\nu), \tag{4}$$

where Γ_D is the Doppler half-width, Γ_0 and Δ_0 are, respectively, the pressure-induced broadening and shift, Γ_2 and Δ_2 are the parameters that quantify the speed dependence of the broadening and shift, ν_{VC} is the frequency of VC collisions, η is the correlation parameter and $\Delta\nu$ is the detuning from the line center, ν_0, at zero pressure.

The limited reliability of the description of VC collisions given by Eq. (1) and adopted in the HTP can be improved by correcting ν_{VC} in the way proposed in Ref. [15]. Here, we follow this approach by replacing ν_{VC} in Eq. (4) with ν_{VC} multiplied by a simple analytical function of the ν_{VC}/Γ_D ratio. This function, called the β correction, is chosen to make the HTP as close as possible to a profile in which the VC collisions are described by a much more realistic BB model (Eq. (2)). We determine the β-correction function for a wide range of perturber-to-absorber mass ratios α.

The β correction is determined as follows. The SDBBP [18] and the HTP are simulated in a wide range of pressures corresponding to $\chi = \nu_{VC}/\Gamma_D$ from 0.01 to 100 and to α from 0 to 5. We limit our study to $\alpha = 5$ as it covers most of the mass ratios of typical atmospheric systems. For the calculations of the reference SDBBP we use the diagonalization [18,30–33] and iterative [34] approaches. Following Ref. [15] we simulate the SDBBP and HTP with the same set of the line-shape parameters, setting Γ_0, Δ_0, Γ_2, Δ_2 to zero, keeping Γ_D constant and varying $\nu_{VC} = \chi \cdot \Gamma_D$. Afterwards, the SDBBP and HTP simulated in this way are compared. In order to best reproduce the SDBBP by the HTP we fit the value of ν_{VC} in the HTP. In these fits, we minimize the maximum absolute value of the difference between the two profiles: |SDBBP − HTP|. This procedure is repeated to cover the considered here ranges of χ and α. Subsequently, we find values of $\beta_\alpha(\chi)$ defined as the ratio of ν_{VC} fitted in the HTP to the original ν_{VC} used in the simulations with the SDBBP.

Determination of the β correction is performed including only the Doppler broadening and velocity-changing collisions, in order to get a universal β-correction function, which is independent of the differences in collisional dephasing affecting various molecules and lines. It was shown in Ref. [15], that when Γ_0, Δ_0, Γ_2, Δ_2 are different from zero, the β-corrected HTP gives a significantly better approximation of the SDBBP than the ordinary HTP. We call the β-corrected HTP simply the βHTP. We propose to use the βHTP in which ν_{VC} in the HTP is replaced by $\beta_\alpha(\chi)\nu_{VC}$ as an approximation of the SDBBP:

$$SDBBP(\ldots, \nu_{VC}, \ldots) \approx \beta HTP(\ldots, \nu_{VC}, \ldots) = HTP(\ldots, \beta_\alpha(\chi)\nu_{VC}, \ldots). \tag{5}$$

As the BB collision operator depends on the mass ratio of colliding molecules, we model the β correction as a mass ratio function. In Fig. 1, a comparison between the simulated SDBBP and HTP with and without the β correction is shown. A full dot, for a given χ and α, is obtained by taking the maximum of the absolute value of the difference between the simulated profiles (|SDBBP − HTP|) and divided by the HTP value at its maximum. Open dots show the same difference but in the case when the value of ν_{VC} in the HTP is adjusted in a way to make the βHTP as close as possible to
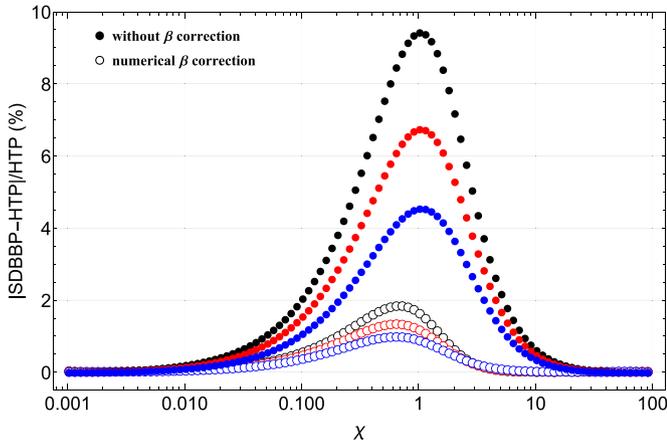
Fig. 1. Dependence of the maximum of the absolute value of the difference between simulated profiles |SDBBP-HTP| divided by the HTP value at its maximum on $\chi = \nu_{\mathrm{VC}}/\Gamma_{\mathrm{D}}$. Full dots show the results for the HTP without the β correction and open dots show the results for the HTP with the β correction. Black, red and blue colors correspond to calculations for $\alpha = 0.1$, 1.0 and 2.5, respectively (note logarithmic scale of horizontal axis). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 2. *Upper panel*: The analytical β-correction function given by Eq. (6) is plotted as black lines (note logarithmic scale of the horizontal axis). Green dots are the numerical calculations of β. Both quantities, χ and α, are dimensionless. The horizontal blue line indicates the correction value taken from Eq. (8), see text for details. *Lower panel*: Relative differences between numerical and analytical values of the $\beta_\alpha(\chi)\nu_{\mathrm{VC}}$ product according to Eq. (5). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the simulated SDBBP. Black, red and blue colors correspond to α equal to 0.1, 1.0 and 2.5, respectively.

The shape of |SDBBP − HTP|/HTP strongly depends on χ: (i) at low χ−the low-pressure limit−the impact of ν_{VC} on the line-shape profile is negligible and the line-shape profile is dominated by the Doppler broadening, (ii) at medium χ−the Dicke narrowing and the Doppler broadening are comparable and the model for the VC collisions plays the most pronounced role, (iii) at high χ−the high-pressure limit−the Dicke narrowing dominates the Doppler width and the line-shape converges to the Lorentz profile [5,8,18], independent of the model for the VC collision operator. In the proposed approach, the application of the β correction in HTP allows a fivefold reduction of the difference between the two profiles in the medium pressure range.

4. Analytical representation of the β correction and its applicability

We introduce the β-correction as a function of two arguments: χ and α, determined in a two-dimensional fitting approach. In the first step, in order to find the best mathematical representation of β with respect to χ for every considered α, we look for a function which best reproduces numerical values of β calculated in the way described in Section 3.

The observed dependence of the β-correction function on χ can be approximated by the following expression:

$$\beta_\alpha(\chi) = A_\alpha \ \tanh(B_\alpha \log_{10}\chi + C_\alpha) + D_\alpha. \tag{6}$$
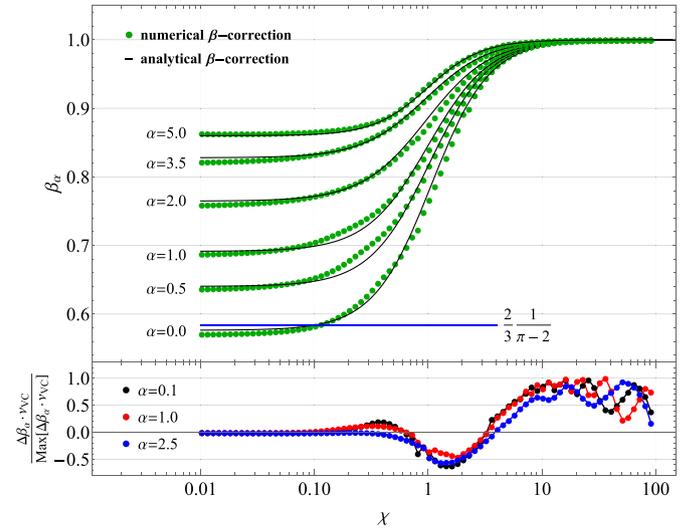
In the second step, this function is independently fitted to numerical values of $\beta_\alpha(\chi)$ for various α in order to find values of parameters. We do it in a way to obtain the smallest difference between the SDBBP and βHTP when applying numerical and analytical values of $\beta_\alpha(\chi)$, see Fig. 4. Next, we determine analytical expressions for each of these parameters, which are provided below:

$$A_\alpha = 0.0534 + 0.1585e^{-0.4510\alpha}, \tag{7a}$$

$$B_\alpha = 1.9595 - 0.1258\alpha + 0.0056\alpha^2 + 0.0050\alpha^3, \tag{7b}$$

$$C_\alpha = -0.0546 + 0.0672\alpha - 0.0125\alpha^2 + 0.0003\alpha^3, \tag{7c}$$

$$D_\alpha = 0.9466 - 0.1585e^{-0.4510\alpha}. \tag{7d}$$

Fig. 2 shows numerical β values (green dots) for χ ranging from 0.01 to 100 and for α from 0 to 5. The black lines correspond to the phenomenological β-correction function. At high χ the β-correction function goes to 1 as at high pressure the VC collisions lead to the same Lorenztian shape of the Doppler component for any reasonable VC colllision operator [5,8,18]. On the other hand, at low χ the β correction converges to the low pressure limit which is different for collisional operators with different α [35]. The lower panel of Fig. 2 shows the relative differences between numerical and analytical values of the $\beta_\alpha(\chi)\nu_{\mathrm{VC}}$ product, which is the quantity entering into the βHTP according to Eq. (5). It is especially important to minimize this differences at higher χ values, in order to minimize the discrepancies between numerical and analytical values of $\beta_\alpha(\chi)$, as shown in Fig. 4. We want to emphasize that the β-correction function is a phenomenological function and it does not have a strict physical meaning. However, it can be seen as a quantity which tells how many hard VC collisions are needed to give a similar effect to BB collisions at given α. Finally, in Fig. 3 we present the functions given by Eqs. (7a)–(7d) for A_α, B_α, C_α and D_α (linear plots) together with numerical values (discrete data points).

In Fig. 4, we demonstrate how well the determined here β-correction function, Eq. (6), is able to improve the HTP. The relative differences between the SDBBP and the βHTP are plotted as open dots when the numerical values of β are taken, and as lines when applying analytical values of β according to Eq. (6). The analytical β-correction function captures well the behavior of numerical calculations. Although the analytical formula performs worse for $\chi > 4$, it still provides a significant improvement over the uncorrected HTP. The presented analytical function is a compromise between the simplicity of mathematical expressions and the agreement with numerical calculations. The β-correction function has been successfully applied in spectral analysis of lines of helium perturbed H$_2$ [36] and of pure D$_2$ lines [37].

In Ref. [38], the relation between the effective frequency of the VC collisions in the soft collision model $\nu_{\mathrm{opt}}^{\mathrm{SC}}$ and in the HC model
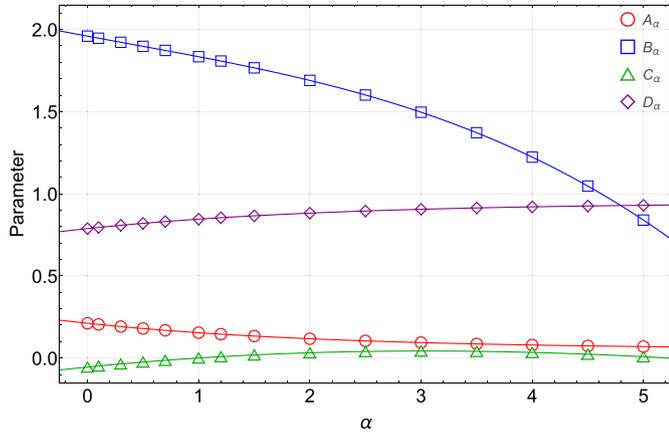
Fig. 3. Overview of the parameters of the β-correction function as a function of α. Numerical values of A_α are plotted as red circles, B_α as blue squares, C_α as green triangles and D_α as purple diamonds. Analytical functions of these parameters, given by Eq. (7a)-(7d), are plotted as lines in corresponding colors. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
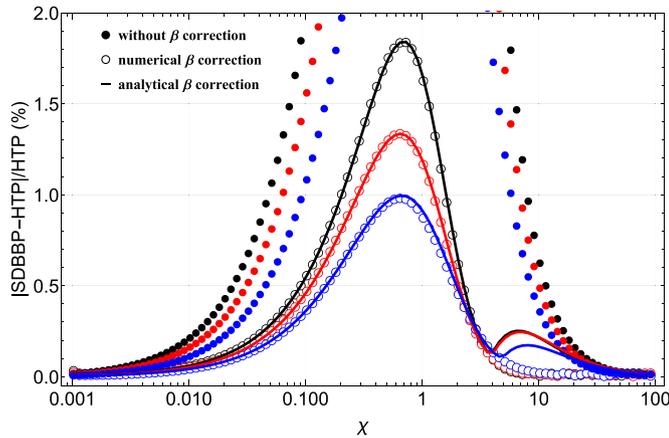
Fig. 4. The relative differences between the SDBBP and the HTP simulated with the same set of parameters (note logarithmic scale of the horizontal axis). This figure partially reproduces Fig. 1. Black, red and blue colors correspond to $\alpha = 0.1$, 1.0 and 2.5, respectively. Open dots represent the difference between the two profiles when numerical values of β are used and lines represent the same difference when analytical β values based on Eq. (6) are applied. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

ν_{opt}^{HC} in the Doppler limit was shown to be

$$\frac{\nu_{opt}^{HC}}{\nu_{opt}^{SC}} = \frac{2}{3}\frac{1}{\pi - 2} \approx 0.584. \tag{8}$$

This relation was derived at low pressure regime from the expression given by Rautian and Sobel'man [8] describing simultaneous influence of the soft and hard collisions on the Doppler broadening. As the soft collisions are eqivuvalent to the BB collisions with $\alpha = 0$, Eq. (8) corresponds to the β correction value at its zero limit, which found numerically equals: $\beta_0(0) \approx 0.576$. This value is about 1.4% lower than the result in Eq. (8), see Fig. 2. This difference is likely a consequence of different approaches to residual minimization used in this work and in Ref. [38]. Here, the residuals were minimized over the entire line, whereas in Ref. [38] only at the maximum residual value.

Calculated values of the β-correction function parameters for selected molecular systems are listed in Table 1. The values were calculated based on Eqs. (7a)–(7d).

Table 1
Values of the β-correction function parameters for selected molecular systems.

System	α	A_α	B_α	C_α	D_α
CO_2-N_2	1.57	0.1314	1.7954	0.0213	0.8686
CO_2-O_2	1.38	0.1384	1.8099	0.0151	0.8616
CO-N_2	1.00	0.1543	1.8444	0.0004	0.8457
CO-O_2	0.88	0.1599	1.8566	-0.0050	0.8401
HF-N_2	0.71	0.1684	1.8749	-0.0131	0.8316
HF-O_2	0.63	0.1726	1.8838	-0.0172	0.8274
HCl-N_2	1.30	0.1415	1.8166	0.0123	0.8585
HCl-O_2	1.14	0.1481	1.8309	0.0062	0.8519
CH_4-N_2	0.57	0.1759	1.8906	-0.0203	0.8241
CH_4-O_2	0.50	0.1798	1.8987	-0.0241	0.8202

5. Conclusions

In this paper a simple analytical correction for the frequency of VC collisions, ν_{VC}, of the HC model adopted in the HTP is presented. The HC model overestimates the frequency of VC collisions in real molecular systems, as it was shown for H_2 perturbed by argon in Ref. [10] or by helium in Ref. [20], as well as in the case of VC collisions described by the Fokker-Planck operator [8,38]. Presented, the β-correction function applied to the HTP reduces the disagreement between the HTP and the more physically justified but more computationally demanding SDBBP [16,18,32] to the percent level, enabling more accurate reproduction of molecular spectra.

In this paper, we propose the β-correction function, which is a function of $\chi = \nu_{VC}/\Gamma_D$ and four heuristic parameters dependent on the perturber-to-absorber mass ratio α. Application of the β correction is of particular significance for studies involving line shapes characterized by a large Dicke narrowing effect and involving multi-spectrum fitting analysis by a line-shape profile assuming the HC model. This correction allows one to maximize the agreement between the HC-based model and experimental spectra with linear dependence of ν_{VC} on pressure. Its implementation does not add any extra fitted parameter and has a negligible influence on the computation time of the line profile.

Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

[1] Ciuryło R, Szudy J. Speed-dependent pressure broadening and shift in the soft collision approximation.. J Quant Spectrosc Radiat Transf 1997;57(1997):411–23. doi:10.1016/S0022-4073(96)00078-7.

[2] Lance B, Blanquet G, Walrand J, Bouanich J-P. On the speed-dependent hard collision lineshape models: application to c_2h_2 perturbed by xe. J Mol Spectrosc 1997;185(1997):262–71. doi:10.1006/jmsp.1997.7385.

[3] Berman PR. Speed-dependent collisional width and shift parameters in spectral profiles. J Quant Spectr Radiat Transf 1972;12(9):1331–42. doi:10.1016/0022-4073(72)90189-6.

[4] Farrow RL, Rahn LA, Sitz GO, Rosasco GJ. Observation of a speed-dependent collisional inhomogeneity in H_2 vibrational line profiles. Phys Rev Lett 1989;63(7):746–9. doi:10.1103/physrevlett.63.746.

[5] Dicke RH. The effects of collisions upon the doppler width of spectral lines. Phys Rev 1953;89(2):472–3. doi:10.1103/PhysRev.89.472.

[6] Galatry L. Simultaneous effect of doppler and foreign gass broadening on spectral lines. Phys Rev 1961;122(4):1218–23. doi:10.1103/physrev.122.1218.

[7] Nelkin M, Ghatak A. Simple binary collision model for van hove's $G_s(r, t)$. Phys Rev 1964;135(1A):A4–9. doi:10.1103/PhysRev.135.A4.

[8] Rautian SG, Sobel'man II. The effect of collisions on the doppler broadening of spectral lines. Sov Phys Uspekhi 1967;9(5):701–16. doi:10.1070/PU1967v009n05ABEH003212.

[9] Tran H, Hartmann JM, Chaussard F, Gupta M. An isolated line-shape model based on the keilson storer function for velocity changes. ii. molecular dynamics simulations and the q(1) lines for pure H_2. J Quant Spectr Radiat Transf 2009;131:154303. doi:10.1063/1.3247898.

[10] Wcisło P, Tran H, Kassi S, Campargue A, Thibault F, Ciuryło R. Velocity-changing collisions in pure H_2 and H_2-Ar mixture. J Chem Phys 2014;141(141):074301. doi:10.1063/1.4892414.

[11] Pine AS. Asymmetries and correlations in speed-dependent dicke-narrowed line shapes of argon-broadened hf. J Quant Spectr Radiat Transf 1999;62(4):397–423. doi:10.1016/S0022-4073(98)00112-5.

[12] Ngo NH, Lisak D, Tran H, Hartmann JM. An isolated line-shape model to go beyond the Voigt profile in spectroscopic databases and radiative transfer codes. J Quant Spectr Radiat Transf 2013;129:89–100. doi:10.1016/j.jqsrt.2013.05.034.

[13] Tennyson J, Bernath PF, Campargue A, Császár AG, Daumont L, Gamache RR, et al. Recommended isolated-line profile for representing high-resolution spectroscopic transitions (IUPAC technical report). Pure Appl Chem 2014;86(12):1931–43. doi:10.1515/pac-2014-0208.

[14] Gordon IE, Rothman LS, Hill C, Kochanov R, Tan Y, Bernath PF, et al. The HITRAN2016 molecular spectroscopic database. J Quant Spectr Radiat Transf 2017;203:3–69. doi:10.1016/j.jqsrt.2017.06.038.

[15] Wcisło P, Gordon I-E, Tran H, Tan Y, Hu S-M, Campargue A, et al. The implementation of non-Voigt line profiles in the HITRAN database: H_2 case study. J Quant Spectr Radiat Transf 2016;177(177):75–91. doi:10.1016/j.jqsrt.2016.01.024.

[16] Blackmore R. A modified Boltzmann kinetic equation for line shape functions. J Chem Phys 1987;87(1987):791–800. 0021-9606/87/140791-10002.10

[17] Lindenfeld M. Self-structure factor of hard-sphere gases for arbitrary ratio of bath to test particle masses. J Chem Phys 1979;73(1979):5817–29. 0021-9606/80/235817-13001.00

[18] Ciuryło R, Shapiro D, Drummond JR, May A. Solving the line-shape problem with speed-dependent broadening and shifting and with Dicke narrowing. II. application. Phys Rev A 2002;65(2002):12502. doi:10.1103/PhysRevA.65.012502.

[19] Ciuryło R, Lisak D, Szudy J. Role of velocity- and speed-changing collisions an speed-dependent line shapes of H_2. Phys Rev A 2002;66(66):472–3. doi:10.1103/PhysRevA.66.032701.

[20] Wcisło P, Thibault F, Cybulski H, Ciuryło R. Strong competition between velocity-changing and phase- or state-changing collisions in H_2 spectra perturbed by ar. Phys Rev A 2015;91(91):052505. doi:10.1103/PhysRevA.91.052505.

[21] Hoang PNM, Joubert P, Robert D. Speed-dependent line-shape models analysis from molecular dynamics simulations: the collision regime. Phys Rev A 2001;65(65):12507. doi:10.1103/physreva.65.012507.

[22] Benner D, Rinsland C, Devi V, Smith M, Atkins D. A multispectrum nonlinear least squares fitting technique. J Quant Spectr Radiat Transf 1995;53:705–21. doi:10.1016/0022-4073(95)00015-D.

[23] Pine A, Ciuryło R. Multispectrum fits of ar-broadened HF with a generalized asymmetric lineshape: effects of correlation, hardness, speed dependence, and collision duration. J Mol Spectrosc 2001;208(2001):180–7. doi:10.1006/jmsp.2001.8375.

[24] Bielska K, Havey, G E Scace DK, Lisak D, Hodges JT. Spectroscopic measurement of the vapour pressure of ice. Phil Trans R Soc A 2012;370:2509–19. doi:10.1098/rsta.2011.0188.

[25] Gotti R, Moretti L, Gatti D, Castrillo A, Galzerano G, Laporta P, et al. Cavity-ring-down doppler-broadening primary thermometry. Phys Rev A 2018;97:012512. doi:10.1103/physreva.97.012512.

[26] Wcisło P, Thibault F, Zaborowski M, Wójtewicz S, Cygan A, Kowzan G, et al. Accurate deuterium spectroscopy for fundamental studies. J Quant Spectr Radiat Transf 2018;213(213):41–51. doi:10.1016/j.jqsrt.2018.04.011.

[27] Liao PF, Bjorkholm JE, Berman PR. Effects of velocity-changing collisions on two-photon and stepwise-absorption spectroscopic line shapes. Physical Review A 1980;21(6):1927–38. doi:10.1103/physreva.21.1927.

[28] Lisak D, Cygan A, Bermejo D, Domenech J, Hodges J, Tran H. Application of the Hartmann Tran profile to analysis of H_2O spectra. J Quant Spectr Radiat Transf 2015;164:221–30. doi:10.1016/j.jqsrt.2015.06.012.

[29] Stolarczyk N, Thibault F, Cybulski H, Jóźwiak H, Kowzan G, Vispoel B, et al. Evaluation of different parameterizations of temperature dependences of the line-shape parameters based on ab initio calculations: case study for the HITRAN database. J Quant Spectrosc Radiat Transf 2019:106676. doi:10.1016/j.jqsrt.2019.106676.

[30] Dolbeau S, Berman R, Drummond JR, May AD. Dicke narrowing as an example of line mixing. Phys Rev A 1998;59(5):3506–12.

[31] Robert D, Bonamy L. Memory effects in speed-changing collisions and their consequences for spectral lineshape: i. collision regime. Eur Phys J D 1998;2(3):245. doi:10.1007/s100530050137.

[32] Shapiro D, Ciuryło R, Drummond JR, May A. Solving the line-shape problem with speed-dependent broadening and shifting and with Dicke narrowing. I. formalism. Phys Rev A 2002;65(2002):12501.

[33] Lisak D, Bielski A, Ciuryło R, Domysławska J, Trawiński RS, Szudy J. On the role of dicke narrowing in the formation of atomic line shapes in the optical domain. J Phys B: At Mol Opt Phys 2003;36:3985–98.

[34] Wcisło P, Cygan A, Lisak D, Ciuryło R. Iterative approach to line-shape calculations based on the transport-relaxation equation. Phys Rev A 2013;88(88):012517. doi:10.1103/PhysRevA.88.012517.

[35] Chandrasekhar S. Stochastic problems in physics and astronomy. Rev Mod Phys 1943;15(1):1–89. doi:10.1103/RevModPhys.15.1.

[36] Słowiński M, Konefał M, Zaborowski M, Jóźwiak H, Nishiyama A, Stolarczyk N, et al. in preparation.

[37] Zaborowski M, Thibault F, Cygan A, Jóźwiak H, Kowzan G, Masłowski P, et al. in preparation.

[38] Wójtewicz S, Cygan A, Masłowski P, Domysławska J, Trawiński R, Lisak D, et al. Spectral line shapes of self-broadened P-branch transitions of oxygen B band. J Quant Spectr Radiat Transf 2014;144(144):36–48. doi:10.1016/j.jqsrt.2014.03.029.