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Temperature dependence of SO_2 line broadening induced by CO_2 in the $\nu_1 + \nu_3$ band

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Sulfur-dioxide line profile parameters at different temperatures are important for the remote sensing of atmospheric gases and monitoring of the environment's state. They are of great importance for monitoring volcanic activity on planets such as Venus and Mars, since their atmospheres consist mainly of carbon dioxide. The work presents the temperature dependence of the broadening coefficients of sulfur dioxide R-branch lines by carbon dioxide pressure in the $\nu_1 + \nu_3$ band. The line widths are calculated in the range of 150−700 K using the semi-empirical method, the parameters of which were obtained as a result of the analysis of experimental data. The temperature exponents are computed using a power law.

Keywords: Line profile parameters, line broadening, temperature exponent, sulfur dioxide, carbon dioxide, Martian atmosphere, Venusian atmosphere.

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1. Introduction

Line profile parameters (broadening and shift coefficients) of sulfur dioxide lines by carbon dioxide pressure are necessary for studying the atmospheres of the Earth and terrestrial planets. They are of primary importance for monitoring volcanic activity, especially on planets such as Venus and Mars, whose atmospheres consist mainly of carbon dioxide (95.3% and 96.5%, respectively) [1–3], while volcanic eruption products contain SO_2 [3–5]. Recent studies of exoplanets predict CO_2 as a dominant atmospheric component [6].

In the Earth's atmosphere [7], sulfur dioxide concentration increases due to anthropogenic activities: besides volcanic activity [8], heavy industry plants contribute significantly to pollution [9]. To study these processes, it is necessary to know not only the line profile parameters (broadening and shift coefficients) but also their distribution over the Earth's atmospheric temperature ranges (200−400 K) [10,11] and those of Venus and Mars (150−700 K) [12,13].

To date, the temperature dependence of sulfur dioxide line broadening by carbon dioxide pressure has been studied only in [{]14 where data were calculated using a semi-empirical (SE) method [15] for the temperature range 150−300 K. SE model parameters were determined based on experimental data [16], and the temperature dependence was obtained using a simple power law. Note that in [14], temperature dependence coefficients were determined only for 41 transitions in the ν_1 band.

In this work, to analyze the temperature dependence of line broadening coefficients in the SO_2−CO_2 system, data were calculated at $T = 150$, 200, 250, 296, 350, 400, 450, 500, 550, 600, 650, 700 K for all transitions of the *R*-branch from [17]. Parameters of the semi-empirical model were previously obtained by us in calculations at room temperature [18,19].

The paper is organized as follows. Section 2 presents the basics of the semi-empirical method and the temperature dependence model. Section 3 shows the calculated temperature dependence parameters, alongside comparison and discussion of results. The final section summarizes the findings and outlines prospects for further research.

2. Theoretical Approach and Computational Details

Calculations of line broadening coefficients for the SO_2−CO_2 system were carried out using the semi-empirical method [15], developed for cases of strong intermolecular interactions. Since the SO_2 molecule is a polar asymmetric molecule with a rather large dipole moment (1.61 D [20]), and the CO_2 molecule is linear nonpolar with a large quadrupole moment of 4.02 DÅ [21], strong dipole-quadrupole interactions occur between them. An effective Hamiltonian model was used to calculate sulfur dioxide energy levels in the ground and (101) states, with spectroscopic constants taken from [22–24].

The semi-empirical method is described in detail in [15], which employs a correction factor —a multiplicative adjustment a correction factor to the interaction efficiency function.. For the SO_2−CO_2 case, the correction factor was chosen as a three-parameter expression:

$$C(JK_a) = \frac{c_1 + c_3 K_a}{c_2\sqrt{J+1}}, \qquad (1)$$

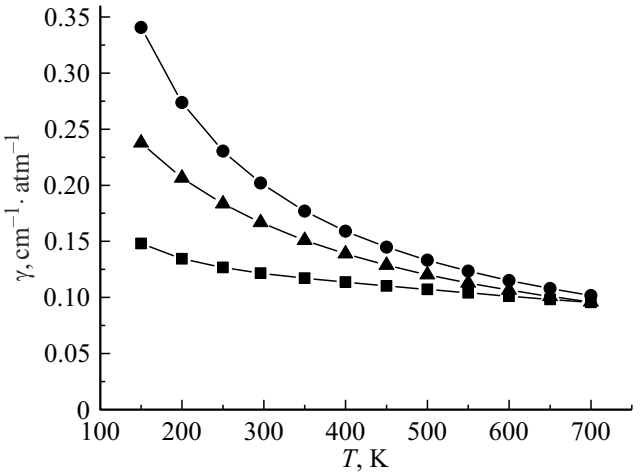

Figure 1. Calculated broadening coefficients for 3 0 3 ← 2 0 2 (circles), 31 10 21 ← 30 10 20 (triangles), 25 18 7 ← 24 18 6 (squares) lines as a function of temperature.

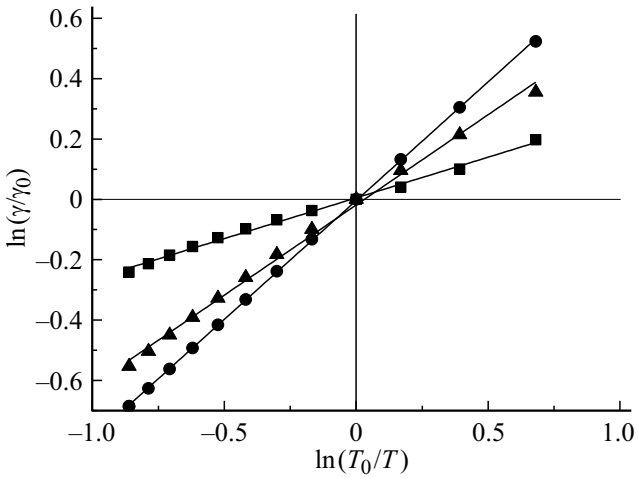

Figure 2. Linear regression of broadening coefficients for SO_2-CO_2 in logarithmic coordinates for lines 3 0 3 ← 2 0 2 (circles), 31 10 21 ← 30 10 20 (triangles), 25 18 7 ← 24 18 6 (squares) in $\nu_1 + \nu_3$ band over the temperature range 150–700 K.

where c_1, c_2, c_3 are adjustable parameters [19]. To determine the semi-empirical model parameters, line widths of the *R*-branch from [17] were selected.

Calculations considered dipole-quadrupole, quadrupole-quadrupole, as well as induction and dispersion parts of the intermolecular potential. The dominant contribution to sulfur dioxide line broadening by carbon dioxide is from dipole-quadrupole interaction, while quadrupole-quadrupole and polarization interactions contribute less than 2 and 0.2%, respectively. Parameters of the intermolecular potential for the sulfur dioxide —carbon dioxide system are given in [19].

To describe temperature dependence of line broadening coefficients for SO_2-CO_2 lines, a simple power law was used, wherein knowing the half-width at a reference temperature and several others allows determination of the temperature exponent using the expression

$$\gamma = \gamma_0 \left(\frac{T_0}{T}\right)^N, \qquad (2)$$

where γ is the broadening coefficient at temperature T, γ_0 is the broadening coefficient at reference temperature $T_0 = 296$ K, and N is the temperature exponent. The value of N is very sensitive to the accuracy of half-width determination, especially for narrow lines: a small error in γ for a narrow line can cause significant uncertainty in N. Note that N does not depend on changes in the correction factor from formula (1). Using this property, parameters of the semi-empirical model determined at room temperature can be used to compute broadening coefficients at other temperatures.

In [25] formula (2) is applied to water line broadening by various buffer gases for temperatures starting from 30 K. It is usually assumed valid over a limited temperature range near $T_0 = 296$ K and it breaks down at low temperatures where semiclassical approach, the use of which assumes the validity of the approximation of classical trajectories of colliding particles, loses its validity. This implies the temperature (i.e., kinetic energy of relative molecular motion) must be sufficiently high to separate translational and internal degrees of freedom. A rough temperature limit criterion is the depth ε of the isotropic intermolecular potential (expressed in kelvins). The lower limit is more of a recommendation than a strict prohibition. For lower temperatures, in absence of advanced quantum calculations with refined potential energy surfaces, this approach may be used.

Maximum N values (observed at low J) agree with so-called „resonance“ contributions of the Anderson–Tsao–Curnutte theory– [26]: $N_{\text{res}} = 0.5 + (n-1)^{-1}$, related to leading dipole-quadrupole ($n = 4$, $N_{\text{res}} = 0.83$) and quadrupole-–quadrupole ($n = 5$, $N_{\text{res}} = 0.75$) interactions in colliding molecule systems. J dependencies for fixed K_a also depend on kinetic and non-resonant terms: $N = N_{\text{res}} + N_{\text{kin}} + N_{\text{nres}}$ [27]. The second term relates to velocity-changing collisions and is expected to be small for active molecules. The last arises from resonance violation and may be negative at low n (e.g., $n = 4$ for water line H_2O broadening by air causing negative temperature exponents [28]). Analyses for N_2O-N_2/O_2 [29] systems and CH_3I-N_2 [30] suggest N_{nres} is mostly due to dipole-quadrupole rather than quadrupole-quadrupole forces.

3. Discussion of Results

To analyze the temperature dependence of SO_2-CO_2 line broadening coefficients by the semi-empirical method, data were calculated at $T = 150$, 200, 250, 296, 350, 400, 450, 500, 550, 600, 650, 700 K for all transitions in the

Temperature dependence coefficients of line half-widths of SO_2-CO_2

ν, cm^{-1}	$J' K_a' K_c' \leftarrow J'' K_a'' K_c''$	N	ν, cm^{-1}	$J' K_a' K_c' \leftarrow J'' K_a'' K_c''$	N
2501.6868	3 2 1 ← 2 2 0	0.693(2)	2507.1605	20 16 5 ← 19 16 4	0.278(11)
2501.7464	3 0 3 ← 2 0 2	0.791(3)	2507.2635	13 5 8 ← 12 5 7	0.736(4)
2502.2152	4 3 2 ← 3 3 1	0.682(5)	2507.2916	16 11 6 ← 15 11 5	0.521(27)
2502.2977	4 2 3 ← 3 2 2	0.696(1)	2507.3156	5 20 5 ← 24 20 4	0.255(13)
2502.8279	5 3 2 ← 4 3 1	0.685(5)	2507.3571	13 0 13 ← 12 0 12	0.698(4)
2502.9293	5 2 3 ← 4 2 2	0.701(1)	2507.4108	14 7 8 ← 13 7 7	0.721(8)
2503.0802	5 1 4 ← 4 1 3	0.762(3)	2507.4208	15 9 6 ← 14 9 5	0.640(20)
2503.1584	6 5 2 ← 5 5 1	0.738(6)	2507.4283	13 4 9 ← 12 4 8	0.726(5)
2503.3134	6 4 3 ← 5 4 2	0.712(8)	2507.4482	17 12, 5 ← 16 12 4	0.462(27)
2503.4089	6 1 6 ← 5 1 5	0.742(4)	2507.5661	18 13 6 ← 17 13 5	0.407(26)
2503.4351	6 3 4 ← 5 3 3	0.690(4)	2507.5939	13 3 10 ← 12 3 9	0.719(3)
2503.5099	6 2 5 ← 5 2 4	0.703(1)	2507.6362	14 6 9 ← 13 6 8	0.737(2)
2503.5709	7 6 1 ← 6 6 0	0.740(3)	2507.6454	19 14 5 ← 18 14 4	0.359(22)
2503.9154	7 4 3 ← 6 4 2	0.713(8)	2507.7122	5 8 7 1 ← 14 8 6	0.688(14)
2503.9440	8 7 2 ← 7 7 1	0.718(10)	2507.7815	4 1 14 ← 13 1, 13	0.679(2)
2504.0399	7 3 4 ← 6 3 3	0.694(4)	2507.8303	14 5 10 ← 13 5 9	0.736(4)
2504.1224	7 0 7 ← 6 0 6	0.767(4)	2507.8401	17 11 6 ← 16 11 5	0.526(26)
2504.2779	9 8 1 ← 8 8, 0	0.677(18)	2507.8456	13 1 12 ← 12 1, 11	0.731(5)
2504.3239	7 1 6 ← 6 1 5	0.760(3)	2507.8495	13 2 11 ← 12 2 10	0.734(2)
2504.3562	8 5 4 ← 7 5 3	0.737(5)	2507.9950	14 4 11 ← 13 4 10	0.730(5)
2504.5124	8 4 5 ← 7 4 4	0.714(7)	2508.0844	14 2 13 ← 13 2 12	0.699(1)
2504.6358	8 3 6 ← 7 3 5	0.7004)	2508.1153	14 3 12 ← 13 3, 1	0.722(4)
2504.6961	8 2 7 ← 7 2 6	0.710(1)	2508.1697	23 17 6 ← 22 17 5	0.272(7)
2504.7578	9 6 3 ← 8 6 2	0.740(3)	2508.1782	20 14 7 ← 19 14 6	0.366(22)
2504.8281	11 10 1 ← 10 10 0	0.560(29)	2508.2137	21 15 6 ← 20 15 5	0.326(17)
2504.8633	10 8 3 ← 9 8 2	0.680(17)	2508.2664	16 8 9 ← 15 8 8	0.689(13)
2504.9476	9 5 4 ← 8 5 3	0.736(5)	2508.3685	15 0 15 ← 14 0 14	0.682(2)
2505.1048	9 4 5 ← 8 4 4	0.716(7)	2508.3833	18 11 8 ← 17 11 7	0.531(25)
2505.1203	10 7 4 ← 9 7 3	0.720(9)	2508.3925	15 5 10 ← 14 5 9	0.737(3)
2505.1527	11 9 2 ← 10 9 1	0.626(23)	2508.5294	19 12 7 ← 18 12 6	0.475(26)
2505.2360	9 3 6 ← 8 3 5	0.704(4)	2508.5645	15 4 11 ← 14 4 10	0.732(5)
2505.2425	9 0 9 ← 8 0 8	0.744(5)	2508.5975	25 18 7 ← 24 18 6	0.265(5)
2505.3437	10 6 5 ← 9 6 4	0.740(3)	2508.6368	20 13 8 ← 19 13 7	0.421(24)
2505.3609	14 13 2 ← 13 13 1	0.374(29)	2508.6818	24 17 8 ← 23 17 7	0.279(7)
2505.4435	11 8 3 ← 10 8 2	0.681(16)	2508.7057	21 14 7 ← 20 14 6	0.374(21)
2505.4608	15 14 1 ← 14 14 0	0.324(24)	2508.7417	18 10 9 ← 17 10 8	0.592(22)
2505.5221	16 15 2 ← 15 15 1	0.283(17)	2508.7525	16 6 11 ← 15 6 10	0.736(2)
2505.6143	13 11 2 ← 12 11 1	0.502(30)	2508.7633	15 3 12 ← 14 3 11	0.725(2)
2505.6501	10 1 10 ← 9 1 9	0.707(5)	2508.8155	17 8 9 ← 16 8 8	0.689(13)
2505.6922	10 4 7 ← 9 4 6	0.718(6)	2508.9212	19 11 8 ← 18 11 7	0.537(24)
2505.7276	12 9 4 ← 11 9 3	0.630(22)	2508.9496	16 5 12 ← 15 5 11	0.738(3)
2505.7867	14 12 3 ← 13 12 2	0.441(30)	2509.0378	15 2 13 ← 14 2 12	0.733(3)
2505.8168	10 3 8 ← 9 3 7	0.709(4)	2509.0670	18 9 10 ← 17 9 9	0.646(18)
2505.8548	10 2 9 ← 9 2 8	0.711(1)	2509.0750	17 7 10 ← 16 7 9	0.720(7)
2505.9244	11 6 5 ← 10 6 4	0.740(3)	2509.0992	26 18 9 ← 25 18 8	0.272(5)
2505.9726	13 10 3 ← 12 10 2	0.570(27)	2509.1181	16 4 13 ← 15 4 12	0.736(5)
2506.0185	12 8 5 ← 11 8 4	0.683(16)	2509.1642	21 13 8 ← 20 13 7	0.428(24)
2506.1787	14 11 4 ← 13 11 3	0.509(29)	2509.1885	25 17 8 ← 24 17 7	0.286(7)
2506.2973	13 9 4 ← 12 9 3	0.633(21)	2509.2289	16 3 14 ← 15 3 13	0.722(3)
2506.3181	11 0 11 ← 10 0 10	0.719(5)	2509.2399	24 16 9 ← 23 16 8	0.309(12)
2506.3458	15 12 3 ← 14 12 2	0.448(29)	2509.2530	23 15 8 ← 22 15 7	0.341(17)
2506.4194	11 3 8 ← 10 3 7	0.713(4)	2509.2798	19 10 9 ← 18 10 8	0.596(21)
2506.4742	16 13 4 ← 15 13 3	0.392(27)	2509.3032	17 6 11 ← 16 6 10	0.735(2)
2506.5000	12 6 7 ← 11 6 6	0.739(3)	2509.4539	20 11 10 ← 19 11 9	0.541(23)
2506.5370	14 10 5 ← 13 10 4	0.576(26)	2509.4632	28 19 10 ← 27 19 9	0.273(6)
2506.5883	13 8 5 ← 12 8 4	0.685(15)	2509.5026	17 5 12 ← 16 5 11	0.739(3)
2506.6272	19 16 3 ← 18 16 2	0.270(11)	2509.6196	18 7 12 ← 17 7 11	0.719(7)

Table. continuation.

ν, cm^{-1}	$J'\,K'_aK'_c \leftarrow J"\,K_a"\,K_c"$	N	ν, cm^{-1}	$J'\,K'_a\,K'_c \leftarrow J"\,K_a"\,K_c"$	N
2506.6343	11 2 9 ← 10 2 8	0.731(1)	2509.7646	24 15 10 ← 23 15 9	0.348(16)
2506.6919	12 5 8 ← 11 5 7	0.736(4)	2509.8083	18 1 18 ← 17 1 17	0.670(3)
2506.7112	11 1 10 ← 10 1 9	0.745(4)	2509.8126	20 10 11 ← 19 10 10	0.599(20)
2506.7293	12 1 12 ← 11 1 11	0.691(4)	2509.8489	18 6 13 ← 17 6 12	0.734(3)
2506.7378	15 11 4 ← 14 11 3	0.515(28)	2509.8982	19 8 11 ← 18 8 10	0.690(12)
2506.8459	13 7 6 ← 12 7 5	0.721(8)	2509.9299	17 3 14 ← 16 3 13	0.728(2)
2506.8529	12 4 (← 11 4 8	0.724(6)	2509.9491	29 19 10 ← 28 19 9	0.279(6)
2506.8617	14 9 6 ← 13 9 5	0.637(21)	2509.9717	17 1 16 ← 16 1 15	0.706(3)
2506.9772	12 3 10 ← 11 3 9	0.716(4)	2509.9813	21 11 10 ← 20 11 9	0.546(23)
2506.9846	12 2 11 ← 11 2 10	0.706(1)	2510.0498	18 5 14 ← 17 5 13	0.741(3)
2507.0706	13 6 7 ← 12 6 6	0.738(3)	2510.0864	28 18 11 ← 27 18 10	0.285(5)
2507.0961	15 10 5 ← 14 10 4	0.580(25)	2510.1114	22 12 11 ← 21 12 10	0.492(23)
2507.1528	14 8 7 ← 13 8 6	0.687(14)	2510.1384	20 9 12 ← 19 9, 11	0.650(16)

Note: ν — Wavenumber (HITRAN [31]), $J'\,K'_a\,K'_c$, $J"\,K"_a\,K"_c$ — rotational quantum numbers of the upper and lower states, respectively, N — temperature exponent. The value in parentheses at N is the standard deviation determined by least squares fitting of line half-widths at different temperatures.

R-branch of the perpendicular $\nu_1 + \nu_3$ band from [17]. The adjustable parameters were determined by us previously in room-temperature calculations [18,19].

Figure 1 shows typical dependencies of line half-widths on temperature changes, exemplified by three lines with small, medium, and large values of the rotational quantum number K_a. It is evident that the broadening coefficients gradually decrease with increasing temperature and approach a constant value.

Fig.2 presents the dependencies of the ratio of γ/γ_0 line half-widths on the ratio of temperatures T_0/T plotted in logarithmic coordinates for a wide temperature range covering atmospheric temperatures of Earth (200−400 K) [10,11], Venus (150−700 K) [12] and Mars (150−300 K) [13]. Negative values on the abscissa correspond to high temperature regions, positive values to low temperature regions. It can be seen that the dependencies in Figure 2 are well described by straight lines whose slopes correspond to the temperature exponents of formula (2). The exponents N were determined by least squares fitting.

Calculated temperature exponents N for the temperature interval$T = 150-700$ K, ordered by increasing transition frequency, are shown in Fig. 3, *a*. Their values range from 0.255 to 0.791. The full dataset can be obtained from the authors; partial data are presented in the table. We grouped all transitions with identical rotational quantum numbers K_a sorted inside each group by increasing quantum number J (Fig. 3, *b*), for example J varies from 2 to 68 at $K_a = 0$, from 10 to 59 at $K_a = 10$, from 24 to 45 at $K_a = 18$. Temperature exponents change smoothly with total angular momentum quantum number for a fixed K_a. Depending on the quantum number K_a temperature dependence coefficients vary significantly: for example, $N = 0.791$ for 3 0 3 ← 2 0 2 line half-width, $N = 0.615$ for 31 10 21 ← 30 10 20, $N = 0.265$ for 25 18 7 ← 24 18 6. The minimal exponent values at large K_a most likely result from a dominant negative contribution from resonance collisions.

Comparison of half-widths reconstructed using formula (2) with those calculated by the semi-empirical method shows good agreement at all temperatures, with an average discrepancy $\sim 1.0\%$ (Fig. 4). The further the temperature is from the reference, the larger the reconstruction error. For instance, the average discrepancy across all transitions is 1.7% at 200 K, 4.0% at 150 K, 0.4% at 400 K, and 1.6% at 700 K. Deviations at 150 and 700 K can reach up to 15.8% and 6.3%, respectively. At 200 K discrepancies greater than 5% (maximum 6.8%) are found only for 25 (out of 621) transitions. Largest deviations occur for $J = K_a$, $K_a = 8-14$, where lines are relatively narrow. These are characterized by relatively small temperature exponents and large standard deviations obtained by least squares fitting. Note that for cases with large deviations, the dependencies shown in Figure 2 are not linear over the entire temperature range 150−700 K, but remain linear within a limited range 200−700 K.

Overall, using the power law is sufficient to describe SO_2-CO_2 broadening in the temperature interval 200−700 K, i.e., for Earth's and Venus' atmospheres. For calculating line half-widths at Mars atmosphere temperatures, a more complex temperature dependence model is needed. References [32,33] report different temperature exponents for different temperature intervals. The HITRAN-2016 database [34] introduced four temperature ranges for line profile parameters, while HITRAN-2020 [31] employs a double power law [35]:

$$\gamma = \tilde{c}_1 \left(\frac{T_0}{T}\right)^{N_1} + \tilde{c}_2 \left(\frac{T_0}{T}\right)^{N_2}, \qquad (3)$$

where $\tilde{c}_1$, $\tilde{c}_2$, N_1, and N_2 are fitting parameters. Expression (3) reduces to the single power law (2) when $\tilde{c}_1 = \gamma_0$, $\tilde{c}_2 = 0$, $N_1 = N$.

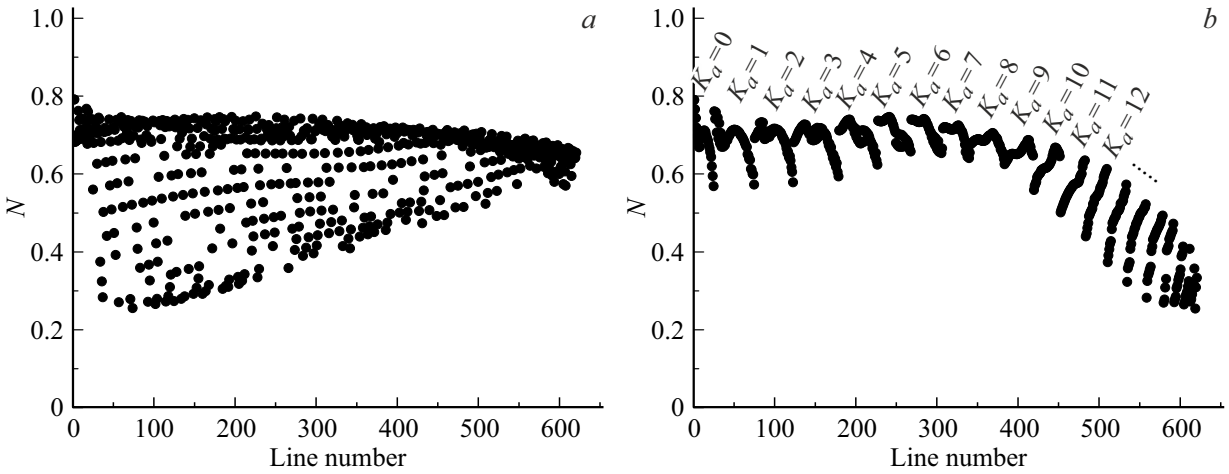

Figure 3. Calculated temperature exponents for line half-widths. Explanations are given in the text.

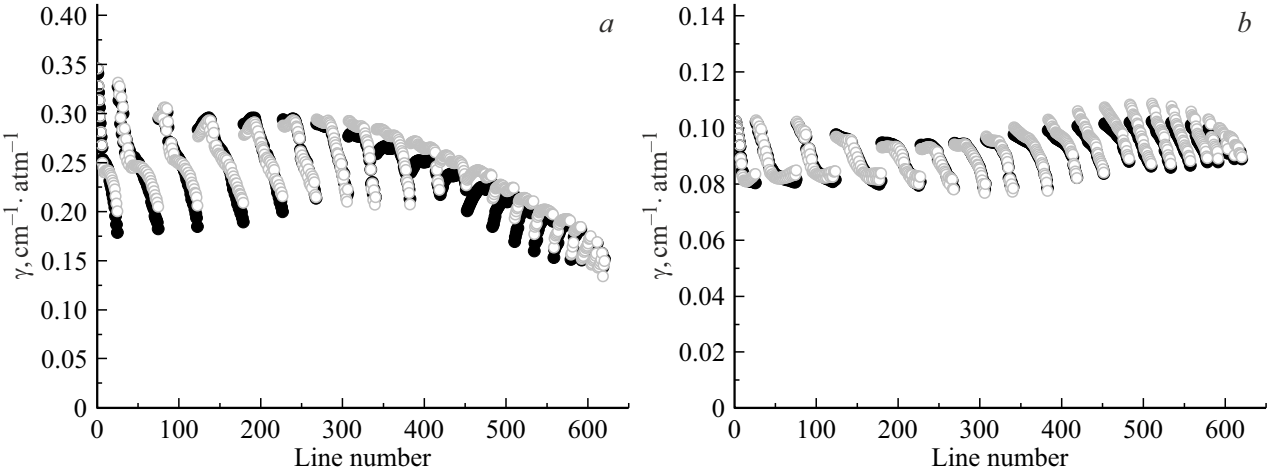

Figure 4. Calculated (filled black circles) and reconstructed (open gray circles) line half-widths at 150 (*a*) and 700 K (*b*).

4. Conclusion

In this work, temperature dependence coefficients of line broadening were calculated for over 600 lines across temperature ranges characteristic of terrestrial planet atmospheres. Calculations employed the power law. Future work plans to use the double power law with four fitting parameters instead of two, allowing better recovery of SO_2-CO_2 line half-widths at low temperatures. It is also foreseen to perform calculations for all transitions of the $\nu_1 + \nu_3$ band presented in HITRAN. Confirmation of the low-temperature calculated values by high-precision experimental data is necessary.

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Conflict of interest

The authors declare that they have no conflict of interest.

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