RATE CONSTANTS OF VT PROCESSES FOR N_2, CO, AND THEIR ISOTOPIC MODIFICATIONS

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Expressions for the rate constants of VT processes are given in the form of a single integral, as well as asymptotic and semiempirical analytical formulas. Calculations are undertaken for N_2 and CO molecules and their isotopic modifications.

In investigating vibrational relaxation in molecular gases, the rate constants are most often calculated using the Landau–Teller formula for the probability of the basic transition with correction formulas taking account of the anharmonism of the vibrations [1, 2] or semiempirical formulas taking account of the deviation of the temperature dependence of the basic-transition probability from the Landau–Teller form [3, 4]. One method of obtaining such semiempirical formulas based on a quasi-classical expression for the T matrix of scattering using action–angle variables for the description of intramolecular motion was proposed in [5-7]. Within the framework of this approach, the influence of attractive forces may be taken into account, without resorting to the mean-energy approximation usually employed in rate-constant calculations [8]; this permits refinement of their low-temperature behavior.

The aim of the present work is to derive analytical approximation formulas of various levels of complexity for the rate constants of VT transfer on the basis of quasi-classical approximation and verification. Calculations for the systems $N_2 + N_2$ and CO + CO and their isotopic modifications demonstrate the sufficiently high accuracy of these formulas and permits their recommendation for use in kinetic calculations.

As discussed in [7], the low-temperature behavior of the rate constants is influenced basically by two factors: the presence of intermolecular attraction and change in the rate of relative translational motion determined by the resonance defect $\Delta E = E_{in_f} - E_{in_i}$, where E_{in_k} is the internal energy of the molecule in channel k (initial i or final f). For most diatomic molecules in the VT-transfer process of interest here, the latter effect is much more significant in view of the large resonance defect $|\Delta E| \gg D$. The temperatures at which the change in translational energy has a pronounced influence on the form of the rate constant of the VT process lie below the value [7]

$$T_\Delta = [(-2\mu\Delta E)^{1/2} + 4(2\mu D)^{1/2}/(3\pi)]^3/(k_B\mu a_f),$$

$$a_k = \pi\mu d l\omega_{nk},\ \omega_{nk} = \omega_e\left[1 - 2x_e\left(n_k + \frac{1}{2}\right)\right],\ k = i,\ f. \tag{1}$$

(So as to be specific, the deactivation process $n_i = n + \ell \to n_f = n$ with $\Delta E < 0$ is considered.) The elastic interaction is modeled by the Morse potential

$$V(R) = D\left\{\exp\left[-\frac{2(R-R_0)}{d}\right] - 2\exp\left[-\frac{R-R_0}{d}\right]\right\}.$$

Taking account of the intermolecular attraction and the change in translational energy on passing from channel to channel in calculating the VT-transition probability leads to the expression for the equilibrium rate constant of deactivation [7]

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$$K_{n_i n_f}(T) = \frac{\tau^{-1}}{N} \frac{2A_f}{B_f} \int_0^\infty e^{-\varepsilon} f(\varepsilon;\ \varepsilon_*,\ D_*)\, d\varepsilon, \tag{2}$$

$$f(\varepsilon;\ \varepsilon_*,\ D_*) = \sqrt{\varepsilon}\,(\varepsilon + \varepsilon_*) \exp\left\{- \frac{B_f}{\sqrt{\varepsilon + \varepsilon_*}} \operatorname{arctg} \sqrt{\frac{\varepsilon + \varepsilon_*}{D_*}}\right\} \times$$

$$\times \left[\operatorname{arctg} \sqrt{\frac{\varepsilon + \varepsilon_*}{D_*}} - \sqrt{\frac{\varepsilon + \varepsilon_*}{D_*}} \Big/ \left(1 + \frac{\varepsilon + \varepsilon_*}{D_*}\right)\right]^{-1},$$

$$A_k = \frac{G^l_{vk}}{\Gamma^2(l+1)} \left[\frac{\pi d}{4\hbar} \left(a_r \omega_{nk} \mu d - (2a_a - a_r) \sqrt{2\mu D}\right)\right]^{2l},$$

$$G_{vk} = n_k + \frac{1}{2} - x_e \left(n_k + \frac{1}{2}\right)^2, \quad \varepsilon_* = -\Delta E / k_\mathrm{B} T'$$

$$D_* = D / k_\mathrm{B} T, \quad B_k = \frac{2a_k}{\pi \sqrt{2\mu k_\mathrm{B} T}}, \quad k = i,\ f.$$

The frequency of elastic collisions τ^{-1} was calculated in [9]. The integration in Eq. (2) is taken over the dimensionless translational energy in the initial channel $\varepsilon = E_i / k_B T$.

As shown in [7], the rate constant of the VT process is close to the Landau–Teller form when $T > T_\Delta$. The integral expression in Eq. (2) is simplified by the usual method here (within the framework of the Laplace method); taking account of the change in translational energy on transition from channel to channel and the intermolecular attraction, this gives [7]

$$K_{n_i n_f}(T) = \frac{\tau^{-1}}{N} \left(\frac{4\pi^5}{27}\right)^{1/6} A_f {B_f}^{1/3} (1 + \xi)^{5/2} \left[1 - \frac{(4/\pi)^{2/2} \varepsilon_*}{B_f^{2/3} (1 - \xi)(1 + y_\Delta)}\right]^{1/2} \times$$

$$\times \exp\left\{-3 \left(\frac{\pi}{4} B_f\right)^{2/3} (1 - \xi) + \varepsilon_*\right\}, \tag{3}$$

$$\xi = \frac{8}{3\pi^2} \frac{\sqrt{D_*}}{B_f}, \quad y_\Delta = \frac{6\varepsilon_*}{\pi^2 B_f^2}.$$

The interpolational coefficient y_Δ is introduced in the corresponding asymptotic formula with the aim of "correcting" its behavior at $T \sim T_\Delta$, where the asymptote ceases to be valid, and "matching" Eq. (3) with the low-temperature constant given below. The circumstance leading to the isolation of the low-temperature constant is associated with taking account of the change in translational energy in the collision process. The Landau–Teller energy E_{LT} at which the integrand in Eq. (2) reaches a maximum – determined, as usual, without taking account of the pre-exponential factor in Eq. (2) is reduced here by $|\Delta E|$ and, with reduction in temperature, passes beyond the limit of integration. Taking account of the pre-exponential factor is insignificant when $T > T_\Delta$ but, when $T < T_\Delta$, it becomes the determining factor. Whereas $E_{LT} \sim T^{2/3}$ at high temperatures, $E_{LT} \sim T$ at $T < T_\Delta$. This leads to change in the dependence of the constant on both the temperature and the quantum numbers. In the low-temperature limit, the dependence on T appears only through the elastic-collision frequency τ^{-1}. This may also be understood from the following considerations. As $E_i \to 0$, the energy in the final channel tends to a finite value ($E_F \to |\Delta E|$) and the transition probability determined by the state parameters in the final channel does not vanish, but tends to a constant value independent of the collision energy. As a result, the integral in Eq. (2) does not depend on the temperature. Finally, at $T < T_\Delta$, the following asymptotic expression is obtained from Eq. (2)

$$K_{n_i n_f}(T) = \frac{\tau^{-1}}{N} \sqrt{\frac{8}{\pi}} \frac{A_f}{B_f} \varepsilon_* \left(1 + \frac{1}{4\varepsilon_*}\right)^3 \times$$

$$\times \exp\left\{-\frac{1}{2} - \frac{2\pi B_f \sqrt{\varepsilon_*} \left(1 + 4\varepsilon_* - 8\sqrt{\varepsilon_* D_*}/\pi\right)}{(1 + 4\varepsilon_*)^2}\right\}. \tag{4}$$

Like the integral expression in Eq. (2), Eqs. (3) and (4) allow the whole matrix of rate constants of VT deactivation for transitions by an arbitrary number of quanta ℓ to be considered.

As an example, these formulas are used to calculate the rate constants of the processes

TABLE 1. Rate Constants $K_{n+1,n}(T)$, cm^3/sec, of the Process in Eq. (5)*

n	T, K												T_Δ, K
	150	200	300	400	500	700	1000	1500	2000	3000	4000	6000	
0	2,5	0,50 0,20	0,24 0,08	0,12 0,060	0,047 0,040	0,050 0,070	0,069 0,11	0,14 0,22	0,11 0,20	0,18 0,27	0,11 0,13	0,12 0,10	198
1	9,4	1,9 0,42	0,92 0,19	0,44 0,15	0,18 0,090	0,19 0,16	0,25 0,26	0,50 0,53	0,39 0,46	0,61 0,60	0,38 0,28	0,42 0,18	197
2	2,0	4,0 0,62	2,0 0,31	0,93 0,26	0,38 0,17	0,39 0,30	0,52 0,47	1,0 0,93	0,77 0,78	1,2 1,0	0,73 0,46	0,78 0,27	196
3	3,5	7,2 0,90	3,5 0,50	1,7 0,47	0,67 0,30	0,67 0,49	0,89 0,77	1,7 1,5	1,3 1,2	1,9 1,5	1,2 0,66	1,2 0,37	195
4	58	12,0 1,2	5,8 0,74	2,7 0,74	1,1 0,47	1,1 0,76	1,4 1,2	2,5 2,1	1,9 1,7	2,9 2,0	1,7 0,90	1,8 0,48	194
5	90	19 1,7	9,0 1,1	4,2 1,1	1,7 0,71	1,6 1,1	2,1 1,7	3,8 3,0	2,8 2,4	4,0 2,8	2,4 1,2	2,4 0,59	193
6	140	28 2,2	14 1,6	6,3 1,7	2,5 1,0	2,4 1,7	3,1 2,5	5,4 4,2	3,9 3,2	5,5 3,7	3,2 1,5	3,2 0,71	192
7	200	41 3,2	20 2,6	9,3 2,5	3,7 1,5	3,5 2,4	4,3 3,4	7,5 5,7	5,3 4,1	7,4 4,6	4,3 1,8	4,2 0,84	191
8	290	60 4,2	29 3,8	14 3,7	5,3 0,22	5,0 3,3	6,0 4,7	10 7,5	7,2 5,4	9,7 5,7	5,5 2,2	5,3 0,97	190
19	12000	2400 120	1200 160	500 140	180 78	145 130	1,4 1,9	190 180	110 65	118 35	57 9,7	44 2,9	178
	—22	—21	—20	—19	—18	—17	—16	—15	—14	—13	—12	—11	

*First row: calculation by Eq. (2); second row) trajectory calculation [10]. The bottom line indicates the order of magnitude of each column.

$$^{14}N_2(n+1) + {}^{14}N_2 \rightarrow {}^{14}N_2(n) + {}^{14}N_2, \tag{5}$$

$$^{12}C^{16}O(n+1) + {}^{12}C^{16}O \rightarrow {}^{12}C^{16}O(n) + {}^{12}C^{16}O \tag{6}$$

and the results are compared with the data of trajectory calculations [10, 11]. Despite the widespread use of the trajectory method, it has a series of deficiencies.

Above all, the calculation results are sensitive to the method used in approximating the potential surface, especially close to the points of rotation [12]. The accuracy of such calculations falls significantly on reducing the temperature. Thus, on taking account only of the short-range potential, the error in determining the constant at 100 K is 100% [11]. In addition, these calculations employ the mean-energy approximation, which is inadequate at low temperatures. All this permits the conclusion that calculations of the rate constants from Eq. (2) at temperatures $T < T_\Delta$ are more reliable.

The results of calculations for $^{14}N_2$ with parameters of the potential $D = 3.58 \cdot 10^{-4}$ at. units, $d = 1.15$ at. units, $a_r = a_a = 0.20$ are shown in Table 1, and results for $^{12}C^{16}O$ with $D = 3.48 \cdot 10^{-4}$ at. units, $d = 1.0$ at. units, $a_r = a_a = 0.1097$ in Table 2. The values of the spectroscopic constants of the molecules used in the calculations are shown in Table 3. The integral in Eq. (2) is calculated from the Laguerra quadrature formula [13] using a ten-point approximation. As is evident from analysis of the data in the tables, the use of Eq. (2) allows sufficiently accurate data to be obtained on the rate constants of VT processes in a wide range of temperatures and quantum numbers, especially if it is taken into account that the results of [10, 11] at $T \gtrsim 1000$ K are somewhat higher than the experimental data. The divergence in the rate-constant values is associated above all with difference in the potential surfaces used in [10, 11] and in the present calculations. Calculation shows that the use of extremely complex surfaces [10, 11] is not justified in terms of the reproduction of the temperature dependence of the constants (as already noted, the discrepancy at low temperatures is associated with the use of the mean-energy approximation in [10, 11] and not with the model of the interaction). On the other hand, taking only the term which is linear with respect to the vibration amplitude in the molecular-interaction potential into account in the calculations leads to a fairly strong dependence on the quantum numbers.

The difference in the data obtained within the framework of Eq. (2) and the asymptotic Eqs. (3) and (4) is apparent mainly in the low-temperature region. This is because Eq. (4)

TABLE 2. Rate Constants $K_{n+1,n}(T)$, cm^3/sec, of the Process in Eq. (6)*

n	T, K											
	150	200	300	400	500	1000	1500	2000	3000	4000	6000	T_Δ, K
0	0,13 0,002	0,23 0,025	0,080 0,067	0,028 0,043	0,087 0,14	0,53 0,33	0,66 0,69	0,38 0,81	0,41 1,2	0,20 0,42	0,16 0,12	220
1	0,48	0,85 0,063	0,29 0,17	0,10 0,11	0,31 0,35	1,9 0,79	2,3 1,6	1,3 1,8	1,4 2,6	0,67 0,91	0,52 0,26	219
2	0,98	1,7 0,12	0,60 0,32	0,20 0,20	0,63 0,66	3,7 1,4	4,5 2,8	2,5 3,1	2,6 4,2	1,2 1,5	0,96 0,42	218
3	1,7	2,9 0,20	1,0 0,53	0,35 0,33	1,1 1,1	6,1 2,3	7,3 4,3	4,1 4,7	4,1 6,2	1,9 2,1	1,5 0,60	216
4	2,6	4,6 0,31	1,6 0,81	0,55 0,51	1,7 1,7	9,4 3,5	11 6,2	6,0 6,6	6,0 8,5	2,8 2,9	2,1 0,79	215
5	3,9	6,9 0,46	2,4 1,2	0,81 0,75	2,5 2,5	14 5,1	16 8,6	8,4 8,8	8,3 11	3,8 3,7	2,8 0,99	214
6	5,6	9,9 0,66	3,5 1,7	1,2 1,1	3,6 3,5	19 7,2	21 12	11 12	11 11	5,0 5,6	3,6	213
7	7,9	14 1,0	4,9 2,4	1,7 1,5	5,0 5,0	26 10	29 15	15 15	14 17	6,4 5,6	4,6 1,4	212
9	15	27 1,9	9,3 4,7	3,1 2,9	9,4 9,0	46 18	50 24	26 22	23 25	10 7,7	7,0 1,9	210
11	27	49 3,5	17 8,5	5,7 5,3	16 17	79 32	82 38	41 31	36 33	15 10	10 2,4	207
19	250	460 34	160 72	51 43	140 140	550 220	490 160	220 86	170 58	64 15	37 3,3	198
29	3600	6700 411	2300 731	690 415	1800 1300	5200 1900	3700 800	1500 220	900 80	300 17	150 3,4	185
	—19	—19	—18	—17	—17	—16	—15	—14	—13	—12	—11	

*Structure as in Table 1.

TABLE 3. Spectroscopic Parameters of Isotopic Modifications of the N_2 and CO Molecules

Isotope	$^{14}N_2$	$^{14}N^{15}N$	$^{15}N_2$	$^{12}C^{16}O$	$^{12}C^{18}O$	$^{13}C^{16}O$	Order of magnitude
ω_e (at. un.)	1,075	1,057	1,038	0,9886	0,9648	0,9666	—2
x_e	6,126	6,126	6,126	6,124	5,977	5,988	—3

is obtained under the assumption that $T \ll T_\Delta$ ($T < 100$ K for the given systems) and poorly reproduces Eq. (2) at $T \sim T_\Delta$ (for the given systems, $T_\Delta \sim 200$ K). Note also that, in accordance with the available experimental data – see [3], for example – the deviation from Landau–Teller conditions for the polar molecule CO is apparent at higher temperatures than for N_2.

The use of the Laguerra quadrature formula in calculating the integral in Eq. (2) permits reduction in the time for the calculation of a single rate-constant value to the time required when using the analytical expressions, and thus the recommendation of Eq. (2) for kinetic calculations.

In connection with [14], the influence of isotopic substitution on the behavior of the VT-transfer rate constants is considered. It is known that N_2 and CO molecules each have two other isotopic modifications other than the basic ones: $^{14}N^{15}N$ and $^{15}N_2$; $^{12}C^{18}O$ and $^{13}C^{16}O$. To study the isotopic effect, the rate constants of the following processes are calculated using Eq. (2)

$$^{14}N\,^{15}N(n+1) + {}^{14}N_2 \rightarrow {}^{14}N\,^{15}N(n) + {}^{14}N_2, \tag{7}$$

$$^{15}N_2(n+1) + {}^{14}N_2 \rightarrow {}^{15}N_2(n) + {}^{14}N_2, \tag{8}$$

$$^{14}N_2(n+1) + {}^{14}N\,^{15}N \rightarrow {}^{14}N_2(n) + {}^{14}N\,^{15}N, \tag{9}$$

$$^{14}N_2(n+1) + {}^{15}N_2 \rightarrow {}^{14}N_2(n) + {}^{15}N_2, \tag{10}$$

$$^{12}C^{18}O(n+1) + {}^{12}C^{16}O \rightarrow {}^{12}C^{18}O(n) + {}^{12}C^{16}O, \tag{11}$$

$$^{13}C^{16}O(n+1) + {}^{12}C^{16}O \rightarrow {}^{13}C^{16}O(n) + {}^{12}C^{16}O. \tag{12}$$

TABLE 4. Numerical Values of the Parameters in Eqs. (13) and (14) for Single-Quantum ($\ell = 1$) Transitions at T_0 = 1000 K

Transition	K_0, cm^3/sec	γ	K_1, cm^3/sec	T_1, K	T_2, K	C
5	0,918	6,515	1,37	1,21	3,39	4,23
6	7,07	5,509	82,6	0,777	3,12	3,52
7	1,01	6,516	1,42	1,19	3,33	4,23
8	1,15	6,511	1,53	1,17	3,27	4,22
9	0,773	6,570	1,02	1,23	3,29	4,26
10	0,655	6,624	0,769	1,25	3,29	4,30
11	7,41	5,534	76,3	0,765	3,04	3,54
12	8,26	5,496	93,1	0,756	3,05	3,51
Order of magnitude	—17	0	—22	7	3	1

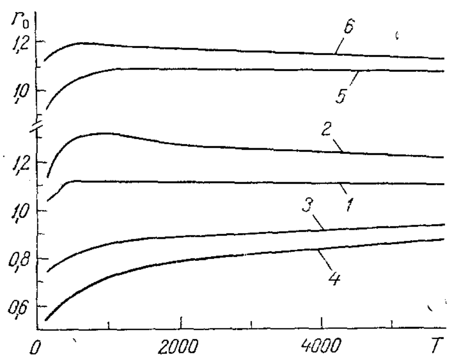

Fig. 1

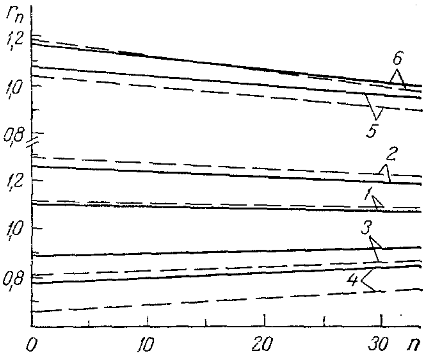

Fig. 2

Fig. 1. Temperature dependence of the isotopic effect for the rate constants of the basic transition in N_2 (curves 1-4) and in CO (curves 5 and 6). T, K.

Fig. 2. Dependence of the isotopic effect on the vibrational excitation of the molecule: 1-4) N_2; 5, 6) CO. The continuous curve corresponds to T = 2000 K and the dashed curve to T = 500 K.

The values of the spectroscopic constants used here are shown in Table 3. Since the isotopic effect is sufficiently small ($\lesssim$40%), the results of these calculations in Figs. 1 and 2 are shown in the form of the ratio $r_n(T)$ of the rate constants of the processes in Eqs. (7)-(10) to the constant of the process in Eq. (5) (curves 1-4, respectively) and the ratio of the rate constants for Eqs. (11) and (12) to that for Eq. (6) (curves 5 and 6). It is evident from Fig. 1 that the isotopic effect due to the change only in the reduced mass of the colliding molecules appears more strongly at low temperatures and decreases monotonically with increase in T (curves 3 and 4). For the processes in Eqs. (7) and (8) and in Eqs. (11) and (12), the isotopic effect is characterized by the presence of a maximum at temperatures 500-1500 K and a very weak temperature dependence at T $\gtrsim$ 1500 K (curves 1, 2, 5, and 6). The dependence of the isotopic effect on the vibrational excitation of the molecule is practically linear and is shown in Fig. 2 for two temperature values.

In a series of problems where what is important is not the fine details of the nonequilibrium vibrational distribution function but only the description of relaxation of its first moment – the vibrational energy [1-3] – less accurate but much simpler approximations may be used for the rate constants. Such approximations may conveniently be derived on the basis of Eqs. (3) and (4). Taking account of the small anharmonism constant x_e, the pre-exponential factors and exponents in Eqs. (3) and (4) are expanded in terms of x_e, confining attention to the linear approximation. The result of this transformation may be written in the form

$$K_{n+l,n}(T) = \begin{cases} (n+1)^l K_{l,0}^{\text{LT}}(T) \exp\left\{2nx_c\left[\left(\frac{T_1}{T}\right)^{1/3} - \frac{T_2}{T}\right]\right\}, & T > T_\Delta, \\ (n+1)^l K_{l,0}^{\text{low}}(T) \exp\{Cnx_e\}, & T < T_\Delta, \end{cases}$$

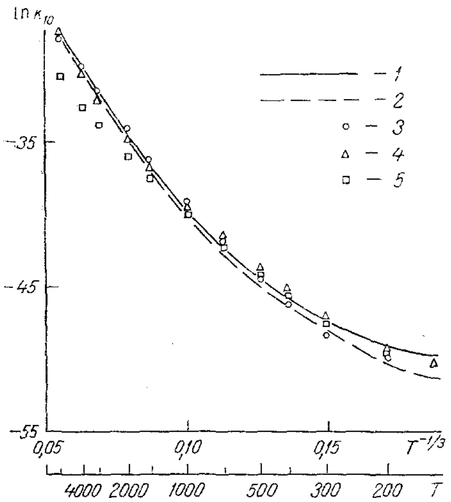

Fig. 3. Temperature dependence of the rate constant of the basic transition for Eq. (5): 1) calculation from Eq. (2); 2) from Eqs. (3) and (4); 3) trajectory calculation [10]; 4) calculation from Eq. (14); 5) from the approximate formula of [4]. ln K_{10}, cm^3/sec; $T^{-1/3}$, $K^{-1/3}$; T, K.

$$T_1 = \frac{\mu}{k_B}(\pi d\omega_e l)^2,\ T_2 = \hbar\omega_e l/k_B,\ C = \pi d(\mu\omega_e l/2\hbar)^{1/2}, \tag{13}$$

and $K_{\ell,0}^{LT}$ and $K_{\ell,0}^{low}$ are the rate constants of the basic transition in Landau–Teller and low-temperature conditions. Thus, Eq. (13) has the characteristic structure for the rate constants of vibrational energy transfer, factorizing into the rate constant of the basic transition, which depends solely on the temperature, and a scale factor which depends on n and T. As is evident from Eq. (13), the scale factor is very simple in form; the expression for $K_{\ell,0}$ is more cumbersome, and may be simplified. To this end, it is sufficient to note that in double logarithmic coordinates, the graph of $K_{\ell,0}^{LT}$ for N_2 and CO molecules is approximated adequately by a straight line. Hence, it is possible to set $K_{\ell,0}^{LT}(T) = K_0(T/T_0)^{\gamma}$, where γ, K_0, and T_0 are fitting parameters. The change in character of the temperature dependence of $K_{\ell,0}$ at $T < T_{\Delta}$ may be taken into account using the term $K_{\ell,0}^{LT}$, which makes a negligible contribution at $T > T_{\Delta}$. Since the temperature dependence at $T < T_{\Delta}$ is weak, this term may be regarded as constant: $K_1 = K_{\ell,0}^{LT}(T_{min})$, where $T_{min} < T$ is the left-hand boundary of the given temperature range. Thus

$$K_{l,0}(T) = K_0(T/T_0)^{\gamma} + K_1. \tag{14}$$

The parameters K_0, T_0, γ may be determined, for example, using the least-squares method from experimental data, the results of trajectory calculations, or data obtained from Eq. (2). Table 4 gives the value of these parameters for single-quantum ($\ell = 1$) transitions in Eqs. (5)-(12) with n = 0 for the temperature range 100-6000 K, with T_0 = 1000 K and the parameters T_1, T_2, and C obtained from Eq. (13).

The rate constant of the basic transition for the process in Eq. (5) calculated from Eq. (14) is compared in Fig. 3 with the results of trajectory calculations, calculations from Eq. (2), and calculations using the approximate formulas of [4]. It is evident from these results that the simple Eq. (14) gives results very similar to those of Eq. (2), is a sufficiently good approximation of the trajectory calculations, and may be recommended for the calculation of the rate constants in a broad range of problems of kinetics and physical gas dynamics. As shown by comparison with the results of trajectory calculations, the conversion formulas in Eq. (13) for the rate constants of transitions between excited vibrational levels cease to operate in the range of n and T where the strong influence of anharmonism of the molecular vibrations begins to be felt. For the CO molecule, for example, this is the region with n $\gtrsim$ 30, T $\gtrsim$ 3000 K, i.e., the region where, in view of the use of the approximation linear with respect to the vibration amplitude in the inelastic intermolecular potential, the results obtained using Eq. (3) differ considerably from the results of trajectory calculations.

NOTATION

E_{in}, internal energy of molecule; D, depth of molecular-interaction potential well; T, temperature; d, radius of action of potential (Morse potential parameter); μ, reduced mass; k_B, Boltzmann constant; ω_e, oscillator frequency; x_e, anharmonicity parameter; n, vibrational level; τ, time of free flight; N, numerical density of gas; K_{nm}, rate constant of transition from level n to level m; $a_{r,a}$, coupling constants in the repulsive and attractive components of the inelastic interaction potential; V(R), molecular-interaction potential.

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