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# Interaction Potential for Vibrational-Translational Energy Transfer in Collision between $I_2^*$ and Ar

By

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## Abstract

In order to determine the interaction potential parameters for vibrational-translational energy transfer collision between Ar and  $I_2^*$  excited by 5145 Å line of an Ar<sup>+</sup> laser, the three dimensional model of Hansen and Pearson is compared with the experimental results of laser induced fluorescence obtained by the method of Steinfeld et al.. In the model, the interaction potential is assumed to be a linear superposition of exponential repulsions between atomic centers and determined by two parameters, i.e., scale size and characteristic length. These are determined to be 0.14 eV and 0.25 Å, respectively, from comparison of the theoretical rate coefficient for the energy transfer with the experimental one relative to their dependence on gas temperature.

## 1. Introduction

Spectroscopy of laser induced fluorescence has presented an interesting and important method to the investigation of energy transfer processes in molecular gases, since a laser can excite specified vibrational-rotational levels of a molecule because of its monochromaticity and high power. One may refer to the review by Demtröder for works in this field up to 1970.<sup>1)</sup>

Iodine molecule is the one that has been most fully investigated in detail, since its  $B^3\Pi_{ou}^+ - X^1\Sigma_g^+$  transition happens to coincide with many visible laser lines, *e.g.*, 6328 Å<sup>2-8)</sup> of He-Ne, 5145 Å<sup>3,6,9-13)</sup> and 5017 Å<sup>6,10,12,14)</sup> of Ar<sup>+</sup>, 5682 Å<sup>5,9,12,15)</sup>, 5308 Å<sup>12)</sup> and 5208 Å<sup>12)</sup> of Kr<sup>+</sup> and 5971 Å<sup>9)</sup> of Xe<sup>+</sup> lasers. Steinfeld and his co-workers have derived, in the series of their papers,<sup>3,10,16,17)</sup> rates of quenching and of vibrational-rotational energy transfers from several specified levels of the *B* state

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of  $I_2$  in the absence or presence of foreign gases by a successive graphical method.

On the other hand, many theoretical calculations of the vibrational energy transfer processes in one and three dimensional models have been reported in the last decade. Excellent reviews in this field up to 1968 have been given by Takayanagi<sup>18)</sup> and Rapp *et al.*<sup>19)</sup>. If a theoretical model is selected on the basis of its qualitative agreement with experimental results, it may be possible to determine the interaction potential parameters included in the model from a quantitative comparison of the dependence of the transition rate coefficients on gas temperature.

In this paper, the experimental method of Steinfeld *et al.* is employed to obtain the rate coefficient for vibrational-translational energy transfer in collision between  $I_2^*$  excited by 5145 Å  $Ar^+$  laser line and neutral Ar under gas kinetic condition, and the dependence of the coefficient on gas temperature is investigated. The results obtained are compared with a calculation based on the model of Hansen and Pearson<sup>20)</sup> to determine the interaction potential parameters under the model.

The interaction parameters between a molecule in the electronic ground state and a colliding particle have been obtained, in most cases, from the vibrational relaxation rates in shock-tubes. In contrast to this, the use of the laser excitation can give information about the electronically excited states of the molecule.

## 2. Experiment

The source of excitation in this experiment was a cw  $Ar^+$  laser, which was operated at a multi-line oscillation at a power level of several tens mW. The 5145 Å and 5017 Å components coincide with the  $B-X$  absorption lines of  $I_2$ . But the laser power of the latter was sufficiently small and only a trace of fluorescence from this origin was observed. Therefore, no special attempt was tried to eliminate the effect of this fluorescence. The assignment of the fluorescence arising from 5145 Å excitation has been done by Steinfeld *et al.*<sup>3)</sup> under a high resolutional condition. It was found that 95% of the fluorescence arises from the absorption in  $P(12)$  and  $R(14)$  branches of  $v'=43 \leftarrow v''=0$  band, while only 5% of it arises from the absorption in  $P(64)$  branch of  $v'=45 \leftarrow v''=0$  band. Therefore, within an accuracy of 5%, the  $v'=43$ :  $J'=11$  and 15 levels of  $B$  state of  $I_2$  are selectively excited by the irradiation of 5145 Å line of an  $Ar^+$  laser.

The experimental setup is shown schematically in Fig. 1. The laser beam was chopped at a frequency of 4 kHz by a rotating chopper. A quartz cell of 20 cm in length and 1.5 cm in diameter had a side arm in which iodine crystals were contained. Temperature  $T$  of the cell was able to be varied from room temperature to 400°C by a nichrom wire heater and measured with a thermo-couple. Iodine of 99.8% purity was distilled into the side arm. The vapor pressure of  $I_2$  was controlled by the

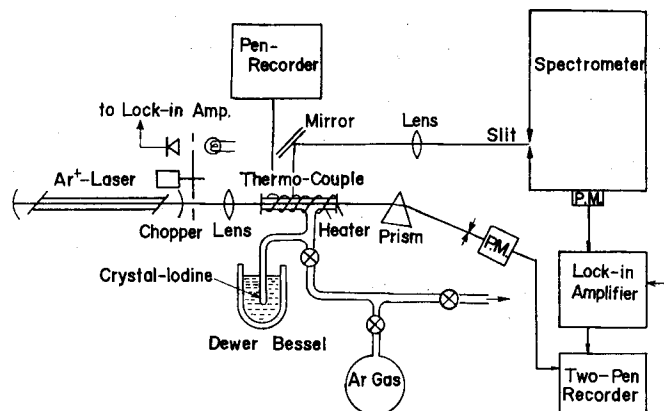


Fig. 1. Schematic diagram of the experimental setup

temperature of the side arm and was determined from the relation obtained by Gillespie and Fraser.<sup>21)</sup> Argon was used as a foreign gas and its pressure was measured with a pirani gauge calibrated by a McLeod gauge. The fluorescence was focused onto the entrance slit of an Ebert type spectrometer of 170 cm focal length, which had the reciprocal linear dispersion of  $4.8 \text{ \AA}/\text{mm}$  in the first order. The light signal was detected by a EMI-6235B photomultiplier and fed into a lock-in amplifier. Incident laser power was monitored by a photomultiplier in order to correct the fluorescence signal for its drift and fluctuation.

An example of the spectra obtained in the absence and presence of Ar is shown

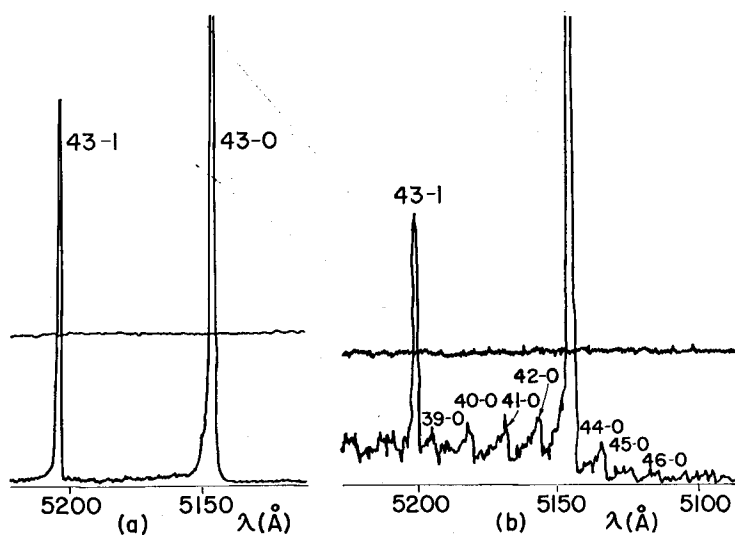


Fig. 2. Fluorescence spectra. (a): in the absence of foreign gas. (b): in the presence of 0.2 Torr of Ar.

in Figs. 2 (a) and (b), respectively. In the former case the fluorescence spectrum was composed of the bands  $v'=43 \rightarrow v''=0, 1, 2, 3$  and 4, which showed the structure  $R(10), P(12), R(14)$  and  $P(16)$  in the observation of high resolution. However, in the latter case, many weak bands appeared, due to vibrational energy transfers.

The procedure to obtain the rate coefficient for vibrational energy transfer is the same as described by Steinfeld *et al.*<sup>10,16)</sup>. The rate coefficients for self and foreign-gas quenchings have to be obtained beforehand. If it is assumed that the quenching rate coefficient and the radiative lifetime are essentially constant for neighboring levels of the  $v'=43$ , each rate coefficient is determined successively by a graphical method.

(i) Self-quenching. If no foreign gas is present in the system, the self-quenching rate coefficient  $Q_s'$  is obtained from the Stern-Volmer equation;

$$I^{-1} = K(M^{-1} + Q_s'). \quad (1)$$

Hereafter, quantities denoted with prime represent the values multiplied by the radiative life time of the level. In the above equation  $I$  is the intensity of any band spectrum arising  $v'=43$ ,  $K$  is a constant and  $M$  is the concentration of  $I_2$ . If one plots  $I^{-1}$  against  $M^{-1}$ ,  $Q_s'$  can be determined from the intersection of the line with the gradient  $K$  to the abscissa. An example of this plot is shown in Fig. 3.

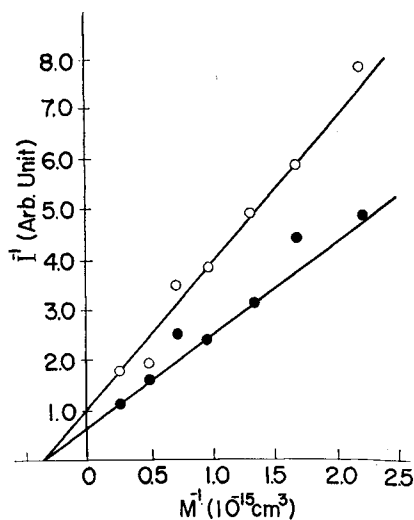


Fig. 3. Plot of eq. (1) for the determination of  $Q_s'$  at  $T=411.0$  K.  $\circ$ :  $I$  is obtained from  $v'=43 \rightarrow v''=2$  band and  $\bullet$ : from  $v'=43 \rightarrow v''=1$  band.

(ii) Foreign-gas quenching. The quenching rate is enhanced when the foreign gas is introduced in the system. Let  $N$  and  $N_0$  be the total populations of  $I_2$  in all  $v'$  levels in the presence and absence of foreign gas, respectively. Then, one obtains the following relation for the rate coefficient of foreign-gas quenching  $Q'$ ;

$$\frac{N_0}{N} - 1 = Q' \frac{X}{1 + Q_s' M}, \quad (2)$$

where  $X$  is the concentration of Ar. If one plots  $N_0/N$  against  $X/(1 + Q_s' M)$  using  $Q_s'$  obtained in the preceding procedure,  $Q'$  can be determined from the inclination of the straight line. An example of this plot is shown in Fig. 4.

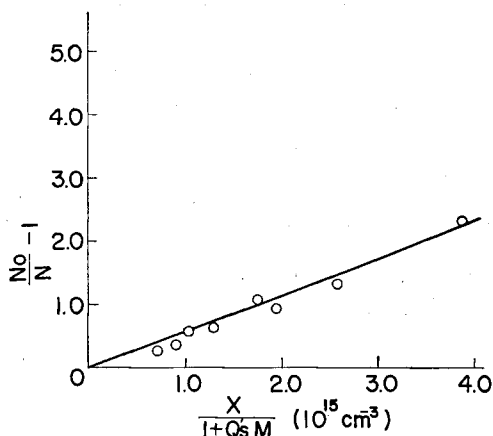


Fig. 4. Plot of eq. (2) for the determination of  $Q'$  at  $T=538.4$  K.

(iii) Vibrational energy-transfer. The rate coefficient of total vibrational transfer out of the  $v'=43$  level  $R'_i$  is obtained from the following relation;

$$\frac{N(43')}{\sum_{v'} N(v') - N(43')} = \frac{1}{R'_i} \left( Q' + \frac{1 + Q_s' M}{X} \right), \quad (3)$$

where  $N(v')$  is the population of the vibrational level  $v'$ , and the vibrational energy transfer from levels  $v' \neq 43$  is neglected. If one plots  $N(43')/(\sum_{v'} N(v') - N(43'))$  against  $(1 + Q_s' M)/X$  as shown in Fig. 5,  $R'_i$  can be determined from the inclination of the straight line. In this plot, the intersection to the abscissa gives  $Q'$ , which must be consistent with the value obtained from eq. (2). In the same manner, the rate coefficient of the specified vibrational quantum jump  $R'(43' \rightarrow v')$  is obtained from the following relation;

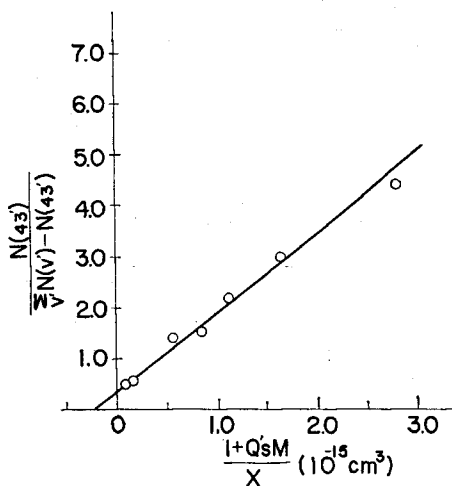


Fig. 5. Plot of eq. (3) for the determination of  $R'_t$  at  $T=293.5$  K.

$$\frac{N(43')}{\sum_{v'} N(v') - N(43')} = \frac{1}{R'(43' \rightarrow v')} \left( Q' + R'_t + \frac{1 + Q_s M}{X} \right). \quad (4)$$

In the plot of eq. (4), one example of which is shown in Fig. 6, the intersection gives  $(Q' + R'_t)$ , which must also be consistent with the preceding results of eqs. (2) and (3). Further, the sum of  $R'(43' \rightarrow v')$  over all  $v'$  must be equal to  $R'_t$ .

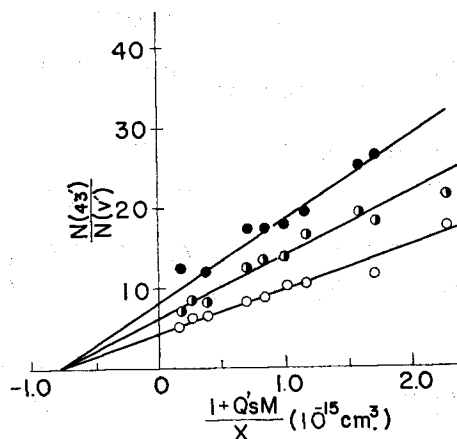


Fig. 6. Plot of eq. (4) for the determination of  $R'(43' \rightarrow v')$  at  $T=411.0$  K.  $\circ$ :  $v'=41$ ,  $\circ$ :  $v'=42$  and  $\bullet$ :  $v'=44$ .

In the above equations from (2) to (4), the population of each vibrational level was obtained from the integrated area of the measured band spectrum divided by

the corresponding Frank-Condon factor. This had been computed by using the computer program of Zare *et al.*<sup>22,23)</sup> with the potentials of  $B$  and  $X$  states given in refs 24 and 25, respectively.

The rate coefficients obtained at five different temperatures  $T$  of the cell are listed in Table I, in which the coefficients are given without prime. The quantities denoted with prime have been divided by the life time of  $v'=43$  level to give the true rate coefficients. Here, the value of  $1.0\mu\text{sec}$  is assumed for this life time.\*

### 3. Calculation

There have been published many theoretical calculations for vibrational-translational energy transfer processes in collisions between an atom and a diatomic molecule. The most conventionally employed model is the semiclassical one. The classical trajectory is assumed for the motion of colliding particles and a time dependent potential perturbation is obtained for the molecule. Then, vibrational transitions produced in the molecule by this perturbation are calculated from quantum mechanics. When this model is corrected for the conservation of the total energy, it becomes as accurate as the first order distorted wave approximation for the collision between heavy particles. This holds true as long as the de Broglie wavelengths of them are much smaller than the scale size of the potential involved.<sup>19,20)</sup>

Table I. Various rate coefficients

rate coeff. ( $\text{cm}^3 \text{sec}^{-1}$ )	$T$ (K)				
	293.5	411.0	462.0	538.4	605.2
$Q_s$	$0.20^{-9}$	$0.36^{-9}$	$0.58^{-8}$	$0.70^{-9}$	$0.75^{-9}$
$Q$	$0.24^{-9}$	$0.45^{-9}$	$0.52^{-9}$	$0.59^{-9}$	$0.76^{-9}$
$R_t$	$0.67^{-9}$	—	$0.90^{-9}$	$0.12^{-9}$	—
$R(43' \rightarrow 41')$	$0.11^{-9}$	$0.13^{-9}$	$0.16^{-9}$	$0.29^{-8}$	$0.37^{-9}$
$R(43' \rightarrow 42')$	$0.17^{-9}$	$0.25^{-9}$	$0.29^{-9}$	$0.47^{-9}$	$0.60^{-9}$
$R(43' \rightarrow 44')$	$0.85^{-10}$	$0.12^{-9}$	$0.13^{-9}$	$0.23^{-9}$	$0.24^{-9}$

The indices give the power of ten by which the values in table must be multiplied.

In this section the semiclassical three dimensional model of Hansen and Pearson<sup>20)</sup> is employed to calculate the rate coefficient for the vibrational-translational energy transfer. The result is compared with the experimental result in the preceding section. In their model, the interaction potential  $U$  between colliding particles is

\* This value is quoted from the consideration of Steinfeld *et al.*<sup>10)</sup> and different from the value of  $2.5 \mu\text{sec}$  estimated by Ezekiel and Weiss<sup>2)</sup> and Chutjian *et al.*<sup>26)</sup>. The use of the larger value will decrease the scale size parameter  $A$  unrealistically as discussed later.



assumed to be a linear superposition of exponential repulsions between atomic centers:

$$U = A[\exp(-r_1/L) + \exp(-r_2/L)], \quad (5)$$

where  $A$  is the scale size of the potential,  $L$  the characteristic length and  $r_1$  and  $r_2$  the distances between a colliding atom and constituent atoms of an harmonic-oscillator molecule. This potential is expanded in terms of first-order influence on the transition probability, and the spherically averaged potential is used to determine the collision trajectory. Then, the time-dependent perturbation derived from this trajectory is applied to the first order perturbation approximation in order to obtain the vibrational transition probability. In this model, vibrational transitions are accompanied by simultaneous rotational transitions. Averaging the probability over collision parameter, the Boltzmann distribution of collision energies and rotational quantum number, one obtains the vibrational transition rate coefficients  $R(v' \rightarrow v' \pm 1)$ ;

$$R(v' \rightarrow v' \pm 1) = \beta^2 \left( \frac{4\pi}{3} \right)^{1/2} \left( \frac{\pi \sigma_0^2}{1 - 2L/\sigma_0} \right)_{x_m} \left( \frac{8kT}{\pi m} \right)^{1/2} \left( \frac{8\pi E_c}{\hbar \omega} \right)^2 \left( \frac{\pi^2 E_c}{kT} \right)^{1/6} \\ \times \exp \left\{ -3 \left( \frac{\pi^2 E_c}{kT} \right)^{1/3} \pm \frac{\hbar \omega}{2kT} \right\}, \quad (6)$$

where

$$\left( \frac{\pi \sigma_0^2}{1 - 2L/\sigma_0} \right)_{x_m} = \frac{\pi L^2 \ln^2 \{ \bar{A} / (\pi^2 E_c)^{1/3} (kT)^{2/3} \}}{1 - 2/\ln \{ \bar{A} / (\pi^2 E_c)^{1/3} (kT)^{2/3} \}}, \\ E_c = m\omega^2 L^2 / 2, \\ \bar{A} = 2A(\sinh \delta / \delta), \\ \delta = \rho_e / 2L, \\ \beta^2 = \beta^2(\Delta v, 0) + \langle R(2) \rangle_{av} \beta^2(\Delta v, \pm 2) + \langle R(4) \rangle_{av} \beta^2(\Delta v, \pm 4), \\ \beta^2(\delta v, 0) = \left( \frac{2}{15} + \frac{\delta^2}{35} + \frac{\delta^4}{630} \right) \left( \frac{\delta^4}{\sinh^2 \delta} \right) \left\langle v \left| \frac{\rho - \rho_e}{2L} \right| v' \right\rangle^2, \\ \beta^2(\Delta v, \pm 2) = \left( \frac{1}{30} + \frac{\delta^2}{105} + \frac{2\delta^4}{2835} \right) \left( \frac{\delta^4}{\sinh^2 \delta} \right) \left\langle v \left| \frac{\rho - \rho_0}{2L} \right| v' \right\rangle^2, \\ \beta^2(\Delta v, \pm 4) = \left( \frac{\delta^4}{22680} \right) \left( \frac{\delta^4}{\sinh^2 \delta} \right) \left\langle v \left| \frac{\rho - \rho_e}{2L} \right| v' \right\rangle^2, \\ \langle R(\Delta l) \rangle_{av} \pm (1 - \lambda^* g)^{7/3} [1 + \pi^{1/2} g \exp(g^2) \{1 + \operatorname{erf}(g)\}] \\ + [1 - \pi^{1/2} g \exp(g^2) \{1 - \operatorname{erf}(g)\}], \\ g = (2B |\Delta l| / \hbar \omega) (\pi^2 E_c / kT)^{1/3} (kT/B)^{1/2}$$

and

$$\lambda^* = (2B|\Delta l|/\hbar)(kT/B)^{1/2}.$$

Here,  $\omega$  is the vibrational frequency,  $\rho_e$  the internuclear distance at the equilibrium of the harmonic oscillator,  $B$  the rotational constant of the simple rotator and  $m$  the reduced mass of the colliding particle.

For the collision between Ar and  $I_2^*$  excited by the 5145 Å laser line,  $I_2^*$  can not be considered to be a harmonic oscillator. Therefore, in this calculation for a one quantum jump,  $\omega$  was determined from the energy difference between the  $v'$  and  $v' \pm 1$  levels,  $\omega = |E_{v'} - E_{v' \pm 1}|/\hbar$ , and the quantity,  $\langle v' | (\sigma - \sigma_e) / 2L | v' + 1 \rangle$ , was calculated numerically by using the computer program of Zare *et al.*<sup>22,23)</sup> for the wave functions of the  $v'$  and  $v' + 1$  levels.

The first order approximation used here is sufficient enough as long as one deals with the transitions of  $\Delta v = \pm 1$ . As for  $\Delta v \neq \pm 1$ , another model, *e.g.*, that of Heidrich *et al.*<sup>27)</sup> which is extended to three dimension by Morse,<sup>28)</sup> may be available.

#### 4. Comparisons and Discussions

The values of  $\bar{A}$ , which determines the scale size of the total potential resulting from both atoms of the molecule<sup>20)</sup>, and  $L$  are determined so as to fit the calculated rate coefficient  $R(43' \rightarrow 42')$  to the one measured at various gas temperatures  $T$ . This is shown in Fig. 7, in which  $R(43' \rightarrow 42')$  is plotted as a function of  $T^{-1/3}$ . The value of  $L$  is determined mainly from the inclination of the plot, and  $\bar{A}$  is obtained from a comparison of the absolute values. The most suitable values of  $\bar{A}$  and  $L$  are

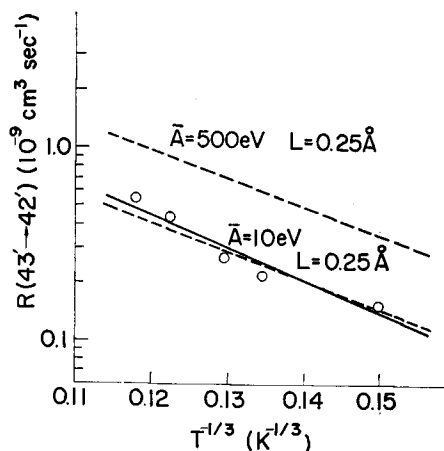


Fig. 7. Dependence of  $R(43' \rightarrow 42')$  on gas temperature  $T$ . —○—: the experimental data. ———: the theoretical calculation.

10 eV and 0.25 Å, respectively. Then,  $A$  is determined from them to be 0.14 eV. Only a little change in  $L$  can largely affect the dependence of the rate coefficient on the gas temperature. Hence, it can be determined with a high accuracy. In contrast to this, a large change in  $\bar{A}$  affects the absolute value of the rate coefficient only slightly. Conversely, if the coefficient is increased only by a factor of 2,  $\bar{A}$  is raised from 10 eV to 200 eV. Such a small change in the rate coefficient may be caused from an experimental error and also from the ambiguity in the life time of  $v'=43$  level. This is the main reason why  $\bar{A}$  (or  $A$ ) can not be determined satisfactorily.

For comparison, the value of  $L$  for the collision between Ar and  $I_2^*$  in the electronic ground state is calculated in the following. In a collision between heavy particles, the Lennard-Jones potential  $U=4\epsilon[(\sigma/r)^{12}-(\sigma/r)^6]$  is often used, which includes two parameters,  $\epsilon$  and  $\sigma$ . The values of  $\sigma$  for Ar—Ar and  $I_2-I_2$  collisions are 3.41 Å<sup>29)</sup> and 4.98 Å<sup>30)</sup>, respectively. For Ar— $I_2$  collision, the combining rule<sup>31)</sup> gives  $\sigma=(3.41+4.98)/2=4.195$  Å in the first order approximation. The Lennard-Jones potential can be fitted to the exponential potential as shown in ref. 19. Then the final result is  $L=0.24$  Å.

In the calculation of the rate coefficient, it has been assumed that the nuclear distance is nearly equal to its equilibrium value, and that  $I_2^*$  is spherically symmetric when it is viewed from the colliding particle. This assumption is not true in the present case, since the 5145 Å laser line excites  $I_2$  to a high vibrational ( $v'=43$ ) and low rotational ( $J'=11, 15$ ) level. In order to carry out a more accurate comparison between calculation and experiment, the use of a tunable dye laser is desirable, which can excite any level of smaller  $v'$  and higher  $J'$ . At the same time, a more accurate measurement of the life time of the excited level must be done, using a short pulse operation of the dye laser.

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