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Deexcitation Probabilities of Ne($^3P_2$) by Ar for the Case E<<D

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Abstract

*The deexcitaion probability calculation of the total Penning ionization cross section for Ne($^3P_2$) by Ar has been made in the region of the collisional energy from 18.5 to 38.1 meV. Comparing the magnitude of the mean collisional energy with respect to D, the application of the analysis in the case E >> D is expected to be more appropriate than in the case E << D. More advance theoretical investigations for Ne($^3P_2$) by Ar should consider the further understanding.***

Keywords: *deexcitation cross sections, collisional energy, pulse radiolysis method, metastable atoms, impact parameter.*

Introduction

Deexcitation processes of excited rare gas atoms play an important role in various phenomena in ionized gases. Penning ionization by long-lived metastable atoms has been intensively studied experimentally.[1-3] The rate constants or the cross sections have been measured by using beam, flowing afterglow, and pulse radiolysis methods. Theoretical investigation has also been reported.[4-6] However, *ab initio* calculations are still limited to some simple cases.[7-11] On the contrary, few experimental works have been reported for the resonance or the radiative states in spite of much theoretical work because of experimental difficulty.[12] Recently, however, several experimental results on the collisional energy dependence of the cross sections for deexcitation of the resonance states have been obtained by the present authors.[13-16]

In this paper, the deexcitation probability calculation of the total Penning ionization cross section for Ne($^3P_2$) by Ar has been made in the region of the collisional energy from 18.5 to 38.1 meV. Comparing the magnitude of the mean collisional energy with respect to potential well depth (D), the application of the analysis in the case E >> D is expected to be more appropriate than in the case E << D.

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Experimental Method and Calculation Procedure

For measuring the deexcitation cross sections a pulse radiolysis method is employed. Details of the apparatus and procedure of the present pulse radiolysis method used for measurements of cross sections for the deexcitation have been described elsewhere.[2,13, 14] It is natural that transition probability P(b) is given in equation (1),

$$\sigma = 2\pi \int_0^{\infty} P(b)bdb \qquad (1)$$

converges to zero or is terminated at a finite maximum impact parameter, b_{max}. Considering the interaction as the source of Penning ionization, the Penning ionization cross section by equation (1) is expressed in a general classical reaction cross section by

$$\sigma = 2\pi \int_0^{b_{\max}} P(b)bdb \qquad (2)$$

Niehaus discussed two particular limits for reducing equation (1) to (2) dependent on the relative amount of a collisional energy E, in comparison with the well depth D of the interaction potential V*(R) as [17]

(1) E << D and E >> D (2)

In the present calculation case (1), i.e., E << D is described. In the case (1) the relative trajectories of a collision are attracted by V* (R), so that the shape of V*(R) strongly alters the amount of P(b). Considering the attractive part of the interaction potential as

$$V^*(R) = -\frac{C}{R^s} \qquad (3)$$

The actual trajectories are affected by the centrifugal barrier emerged on the effective potential

$$V_{eff.}(R) = -\frac{C}{R^s} + \frac{Eb^2}{R^2} \qquad (4)$$

and repelled by the repulsive wall of V_{eff}.(R) of eq.(4) at the classical turning point R_0(b) for V_{eff}.(R_0) = E. However, at a certain b = b_c, $V_{eff.}$(R) = E is also satisfied at the top of the centrifugal barrier giving a classical orbiting trajectory, i.e., radial motion is "frozen" by $dV_{eff.}(R)/dR = 0$. This also implies that R_0(b) jumps from a smaller value around the repulsive wall to a larger value outside of the centrifugal barrier in passing through b = b_c. It is thus a reasonable assumption that the value of P(b) has a considerable amount at b<b_c but drops to almost zero at b = b_c which allows the Penning ionization cross section by eq.(2) written as

$$\sigma = P\pi b_c^2 \qquad (5)$$

for the constant value of P(b) = P at b< b_c. Assuming a dispersion force for the attractive V*(R) between neutral atoms as s = 6, b_c is given by

$$b_c = \left(\frac{3}{2}\right)^{1/3}\left(\frac{3C_6}{2E}\right)^{1/6} \tag{6}$$

where C_6 is the van der Waals coefficient. C_6 can be given by the Slater- Kirkwood equation for dispersion force.[18-20] Thus at the limit of the case (1) the deexcitation (Penning ionization) probability should be obtained as

$$P = \frac{\sigma_M}{\pi b_c^2} \tag{7}$$

However, the reported cross section is thermally averaged over the Maxwellian distribution of f(v) so that in the present analysis[14]

$$P_c = \frac{\sigma_M}{<\sigma_c>} \tag{8}$$

is taken, where

$$<\sigma_c> = \frac{k_c}{<v>} = \int \frac{v\left(\pi b_c^2\right)\mathrm{f(v)dv}}{<v>} \tag{9}$$

Results and Discussion

The reported experimental data are analyzed by considering the case (1), i.e , E << D.[14] For the case (1), the reported deexcitation cross sections, σ_M and deexcitation probabilities, P_c are shown in Table 1.

Table 1: Deexcitation probabilities P_c of Ne($^3P_2$) by Ar for the case (1).

Collisional energy(meV)	38.1	35.3	32.7	30.1	27.5	24.9	22.4	19.8	18.5
σ_{Ar} (Å^2)	13.2±0.4	15.0±1.2	13.1±1.0	13.9±1.1	13.2±1.2	11.3±0.8	12.0±1.0	12.5±1.5	12.6±1.0
P_c	0.15±0.01	0.16±0.01	0.14±0.01	0.14±0.01	0.13±0.01	0.11±0.01	0.11±0.01	0.11±0.01	0.11±0.01

The values of P_c in Table 1 increase gradually with increasing the mean collisional energy for the deexcitation of Ne($^3P_2$) by Ar, which shows that the assumption of P(b) = P (constant) at $b < b_c$ to derive eq.(5) is not appropriate. It is interesting that the region of collisional energy which fills the 0 < E < D coincides with the region where the cross section obtained by cross beam experiments dispersively increased with decreasing the collisional energy.[21] Because the present thermally averaged cross sections are the averaged values of cross sections weighted by the Maxwellian distribution, a small amount of contribution (<10%) of the collisions for 0 < E < D is involved. Considering the magnitude of the mean collisional energy with respect to D, the application of the analysis in the case (2) is expected to be more appropriate than the case E << D. For further understanding of deexcitation of metastable neon atoms, theoretical investigations such as quantum mechanical optical model calculations and *ab initio* calculations of the optical potentials should develop for Ne($^3P_2$) by Ar.

Conclusions

The deexcitaion probablity calculation of the total Penning ionization cross section for Ne($^3P_2$) by Ar has been made in the region of the collisional energy from 18.5 to 38.1 meV. Comparing the magnitude of the mean collisional energy with respect to potential well depth, D, the application of the analysis in the case (2), i.e., E >> D is expected to be more appropriate than in the case E << D. Also the theoretical investigations such as quantum mechanical optical model calculation and *ab initio* calculations of the optical potentials should develop for the further understanding.

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