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Calculation of Deexcitation Probability 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 at collisional energy 38.1 meV. The comparison of d*eexcitation cross sections, polarizability, α / β, deexcitation probability, $\{IP(M)/IP(Ne^*)\}^{1/2}$ and the well depth of interaction potentials for *Ne($^3P_2$) by Ar for the case E >> D has been made.*

Keywords: *deexcitation probability, deexcitation cross sections, collisional energy, pulse radiolysis method, metastable atoms, polarizability, interaction potential.*

Introduction

Penning ionization of atoms and molecules by excited rare gas atoms in metastable states has been extensively studied.[1-4] 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.[5-7] However, *ab initio* calculations are still limited to some simple cases.[8-12] On the other hand, few experimental works have been reported for the resonance or the radiative states in spite of much theoretical work because of experimental difficulty.[13] However, several experimental results on the collisional energy dependence of the cross sections for deexcitation of the resonance and metastable states have been obtained by the present authors.[13-17]

In this paper, the deexcitaion probability calculation of the total Penning ionization cross section for Ne($^3P_2$) by Ar has been made at collisional energy 38.1 meV. The comparison of deexcitation cross sections, polarizability, α / β, deexcitation probability, $\{IP(M)/IP(Ne^*)\}^{1/2}$ and the well depth of interaction potentials for Ne($^3P_2$) by Ar for the case E >> D has been made.

Results and Discussion

The deexcitation cross section has been measured by using a pulse radiolysis method. The experimental apparatus and procedure of the present pulse radiolysis method have been described in detail previously.[3,4,13, 14] It is natural that transition probability P(b) is given in equation (1),

$$\sigma = 2\pi \int_0^\infty P(b) b\,db \qquad (1)$$

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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

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

where P(b) is the transition probability and can be written as

$$P(b) = 1 - \exp\{-2\int_0^{\infty} \mathrm{dR}\Gamma(\mathrm{R})/\hbar\nu(\mathrm{b, R})\} \qquad (3)$$

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 [18]

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

In the present calculation case (2), i.e., E >> D is described. In the case (2) the relative kinetic energy, E is considerably larger than the well depth, D, the influence of the attractive part of V*(R) can be neglected and V*(R) approximated by a pure repulsive potential.
Niehaus proposed that V*(R) is expressed as[2, 18, 19-21]

$$\mathrm{V*(R) = Bexp(-\beta R)} \qquad (4)$$

where B and β are constant.

The autoionization width Γ (R) which is related to the overlap of target orbitals with the 2p vacant orbital of Ne($^3P_2$) increases exponentially with decreasing R. Although a strong anisotropy could be present in Γ (R) depending on the direction of 2p vacancy in Ne($^3P_2$), only the isotropically averaged Γ (R) is considered here.[22,23] The transition probability of an electron-exchange interaction is given by [2, 18, 19-21]

$$\Gamma(R) = \mathrm{A\exp(-\alpha R)} \qquad (5)$$

where A and α are constant. Substituting eqs.(4) and (5) into eq.(3) and then into eq.(1) under the considereation of eq.(2), the cross section can be simplified as[2]

$$\sigma \propto \mathrm{E}^{\alpha./\beta\ -1/2}\{\ln(E/C)\}^2, \qquad (6)$$

which is rewritten more simplified form, if the variation of σ due to a logarithmic part is much smaller than the exponential part, as [2, 18, 19,20]

$$\sigma \propto \mathrm{E}^{\alpha./\beta\ -1/2} \qquad (7)$$

In the present analysis thermal averaging is also taken into consideration as in the case (1). For the case (2), the repulsive "hard core" of the interaction potential determines the trajectrory like in Billiard ball or rigid sphere collision. The deexcitation probability, P_{RS}, are given as the ratios of experimental cross sections to the rigid sphere collision cross sections, σ_{RS}, calculated using Lennard-Jones parameters[24,25], for Ne($^3P_2$)by Ar (58.6 Å^2)

Considering the magnitude of the mean collisional energy with respect to well depth, D, the application of the analysis in the case (2) is expected to be more appropriate. Koizumi et al. similarly analyzed the data for He(^3S)-Ar, Kr, N_2, CO, O_2, CO_2 and C_2H_4 and observed a good correlation

between α / β and P_{RS} .[26] Because the number of target atoms studied in the present experiment is limited only Ar atom.
It was also shown that the ratio α / β is expressed as [18,27-29]

$$\alpha / \beta \cong \{IP(M)/IP(Ne^*)\}^{1/2} \qquad (8)$$

The reported experimental data are analyzed by considering the case (2), i.e , E >> D.[14] For the case (2), the reported deexcitation cross sections, $\sigma_{M,}$ polarizability, α / β, deexcitation probability (P_{RS}), $\{IP(M)/IP(Ne^*)\}^{1/2}$ and the well depth of interaction potentials D are shown in Table 1.

Table 1: *Deexcitation cross sections, $\sigma_{M,}$ polarizability[30], (see text) α / β, deexcitation probability (P_{RS})[18], $\{IP(M)/IP(Ne^*)\}^{1/2}$ and the well depth of interaction potentials, D.[31]*

Target atom	*Deexcitation cross sections* (Å^2)	*Polariz-ability* (Å^3)	α / β	Deexcitation probability (P_{RS})	$\{IP(M)/IP(Ne^*)\}^{1/2}$	Well depth of interaction potentials, D (meV)
Ar	13.2±0.4	*1.64*	0.71±0.06	0.23±0.01	*1.78*	*5.45*

Conclusions

The deexcitaion probability calculation of the total Penning ionization cross section for Ne($^3P_2$) by Ar has been made at collisional energy 38.1 meV. The comparison of deexcitation cross sections, polarizability, α / β, deexcitation probability, $\{IP(M)/IP(Ne^*)\}^{1/2}$ and the well depth of interaction potentials for Ne($^3P_2$) by Ar for the case E >> D has been made. Theoretical investigations for Ne($^3P_2$) by atoms 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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