ArF*, KrF* AND XeF* EMISSIONS PRODUCED FROM DISSOCIATIVE ION RECOMBINATION REACTIONS OF Ar⁺, Kr⁺ AND Xe⁺ WITH SF₆⁻ IN THE FLOWING AFTERGLOW

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The ArF*, KrF*, and XeF* emissions resulting from dissociative ion recombination between rare gas cations and SF_6^- anions have been studied in the flowing afterglow. The anions were formed by thermal electron capture by SF₆. The KrF* product state distribution from the two Kr⁺(²P_{3/2}) spin-orbit states showed that the B and C states are preferentially formed by the Kr⁺(²P_{3/2}) reaction, while Kr⁺(²P_{1/2}) favors formation of the D state. The state selectivity can be explained by consideration of the potential energy diagram.

1. Introduction

There has been a continuous interest in the rare gas halide excimer emissions because of their importance in application to high power lasers. Excimer formation from two-body reactions between metastable rare gas atoms and halogen-containing molecules has been extensively studied by using flowing afterglow (FA) and beam apparatus [1-14]. It is believed that excimer formation proceeds through a curve crossing of a covalent Rg*-RX entrance potential with an Rg⁺-RX⁻ ion-pair potential: the dissociation of the [Rg⁺-RX⁻] intermediate results in the formation of RgX* excimer,

$$Rg^{*} + RX \rightarrow [Rg^{+}RX^{-}] \rightarrow RgX^{*} + R.$$
 (1)

The reaction dynamics has been found to depend upon the properties of the $[Rg^+RX^-]$ intermediate.

The reactions of Ar(${}^{3}P_{0,2}$), Kr(${}^{3}P_{2}$), and Xe(${}^{3}P_{2}$) with SF₆ have been studied in the flowing afterglow [2,3,5]. The total quenching rates for Ar(${}^{3}P_{0}$), Ar(${}^{3}P_{2}$), Kr(${}^{3}P_{2}$), and Xe (${}^{3}P_{2}$) at 300 K were measured to be 1.7×10^{-10} , 1.6×10^{-10} , 1.8×10^{-10} , and 2.3×10^{-10} cm³ s⁻¹, respectively [5]. No RgF* excimer emission has been observed [2,3]. The absence of excimer formation channel was explained as due to the fact that [Rg+SF₆] intermediates predissociate rather than form RgF* excimer [15].

Wren et al. [15] found strong XeF* excimer emission from a Xe/SF₆ mixture in a tesla-coil-driven discharge. Since Xe(${}^{3}P_{2}$) and Xe(${}^{3}P_{1}$) reacting with SF₆ do not give XeF*, the observation of XeF* from SF₆ requires the reactions of Xe** Rydberg states or recombination of Xe⁺ and F⁻ or SF₆⁻ ions. Arguments based upon XeF* vibrational and electronic state populations and the time dependence of the emission suggested that the Rydberg-state reaction was the dominant mechanism contributing to the XeF* excitation. Wren et al. [15] predicted that excimer formation would be an unimportant exit channel in the two-body dissociative recombination of Xe⁺ and SF₆⁻ as in the Xe(${}^{3}P_{2}$)/SF₆ reaction.

Cooper et al. [16] studied the formation of KrF* and XeF* in electron-beam irradiated Kr/Xe/SF₆ mixtures by measuring time-dependent excimer formation and decay. A slow, electron-beam-energy-dependent process has been observed, and attributed to dissociative ion recombination between Kr⁺ or Xe⁺ and SF₆⁻. This observation disagrees with the prediction of Wren et al. described above.

In the present study, ArF*, KrF*, and XeF* emissions have been observed from the FA reactions of SF₆, and confirmed to be due to ion-neutralization processes between rare gas cations and SF₆⁻ anions. The $Kr^+({}^2P_{3/2})$ ion favors the $KrF^*(B, C)$ states, while the $KrF^*(D)$ state is formed with high propensity from the $Kr^+({}^2P_{1/2})$ reaction. The state selectivity is discussed in terms of diabatic potential diagram.

2. Experimental

The FA apparatus used in this study is shown in fig. 1. The metastable He(2 ${}^{3}S$) atoms and the He⁺ and He⁺₂ ions were generated by a microwave discharge of high purity He operated at 0.6–1.8 Torr (1 Torr=133.3 Pa). After trapping the ionic active species by using a pair of grids, the He(2 ${}^{3}S$) atoms flowed downstream past the first gas inlet from which a small amount of the Ar, Kr, or Xe gas was admixed. Ar⁺, Kr⁺, or Xe⁺ in the ground electronic state was produced by Penning ionization:

- $He(2^{3}S) + Ar \rightarrow Ar^{+}(^{2}P_{3/2,1/2}) + He + e^{-},$ (2)
- $He(2^{3}S) + Kr \rightarrow Kr^{+}(^{2}P_{3/2,1/2}) + He + e^{-},$ (3)

$$He(2^{3}S) + Xe \rightarrow Xe^{+}({}^{2}P_{3/2,1/2}) + He + e^{-}$$
. (4)

The rate constants for processes (2)-(4) have been measured as $(7-9)\times10^{-11}$, $(10-14)\times10^{-11}$, and $(12-18)\times10^{-11}$ cm³ s⁻¹, respectively [17]. The branching fraction of the two spin-orbit components, ${}^{2}P_{1/2}/{}^{2}P_{3/2}$, was estimated to be 0.52 for Ar⁺, ≈ 0.56 for Kr⁺, and 0.49 for Xe⁺ from the analysis of Penning ionization electron spectra [18]. The SF₆ gas (purity >99.65%) was injected into the discharge flow through the second inlet placed ≈ 1 cm downstream from the first gas inlet. The partial pressure in the reaction zone was 10–50 mTorr for Ar,



Fig. 1. Schematic representation of the flowing afterglow cell used for the optical study on ion-recombination processes.

Kr and Xe and 5–20 mTorr for SF₆. The emission spectra were observed with a Jarrell-Ash 1 m monochromator in the 180–400 nm region. The observed spectra were uncorrected for the sensitivity of the detection system.

3. Results and discussion

When small amounts of Ar and SF₆ were added to the He discharge flow through the first and second gas inlets, respectively, a broad emission was detected in the 190-280 nm region as shown in fig. 2. By reference to reported data on rare gas excimer [6,10,19], the band in the 190–200 nm region with a structure due to O₂ absorption is ascribed to the (B, $\Omega = 1/2 - X$, $\Omega = 1/2$) transition of ArF*, while that in the 200-400 nm region is assigned to the (C, $\Omega = 3/2 - A$, $\Omega = 3/2$) transition of ArF*. The C-A band has no oscillatory structure and the peak intensity shifts to blue in comparison with those obtained from the Ar*/F2, NF3, CF3OF reactions [6,10]. A similar tendency has been generally found for the C-A emissions of XeCl* [7,8] and XeBr* [9] with high vibrational population at low v' levels. By analogy, it is reasonable to assume that the C state of ArF* is excited in low vibrational levels.

The fairly good agreement of the total quenching rate of $He(2^{3}S)$ by Ar with the ionization rate [17] indicates that Penning ionization leading to Ar⁺ ions is the only product channel in the $He(2^{3}S)/Ar$ re-



Fig. 2. ArF^{*} emission produced from ion recombination between Ar⁺ and SF₆⁻ in the He afterglow (He: 1.6 Torr; Ar: 50 mTorr; SF₆: 10 mTorr). The optical resolution is 3.8 Å (fwhm). The structure of ArF^{*}(B-X) in the 190-200 nm region originates dominantly from the O₂ absorption in the detection system.

action. On the basis of Penning ionization electron spectra [17,18], Ar^+ ions formed through process (2) are located in the ground ${}^{2}P_{3/2}$ and ${}^{2}P_{1/2}$ spinorbit states with recombination energies of 15.76 and 15.94 eV, respectively. The two-body reaction between Ar^+ and SF_6 can be excluded from the possible excitation mechanism because the excimer formation is endoergic by 5.3 eV for $ArF^*(B)$ and by 5.5 eV for $ArF^*(C)$ [19,20]

$$Ar^{+} + SF_{6} * ArF^{*} + SF_{5}^{+}, \qquad (5)$$

$$\rightarrow SF_5^+ + F + Ar , \qquad (6)$$

 $k_6 = 1.2 \times 10^{-9}$ cm³ s⁻¹ [21], 9.3×10^{-10} cm³ s⁻¹ [22]. SF₆ is a good thermal electron scavenger with a large electron attachment rate constant of 2.2×10^{-7} cm³ s⁻¹ [23]. The branching ratio for thermal electron attachment to SF₆ has been measured as SF₆ :SF₅ :F⁻ = 200000:1:0 at 20°C [23], indicating that SF₆ is the only important anion in thermal electron attachment:

$$e^- + SF_6 \to SF_6^- . \tag{7}$$

In the present experiment, SF_6^- must be produced by attachment of Penning electrons generated from process (2) to SF_6 . Summarizing this information, it was concluded that the ArF* emission results from the following ion-neutralization process at thermal energy:

$$Ar^{+} + SF_{6}^{-} \rightarrow ArF^{*}(B, C) + SF_{5}.$$
(8)

When the Ar gas was replaced by Kr or Xe, the KrF* or XeF* excimer band was observed as shown in figs. 3a and 3b. The (B, $\Omega = 1/2 - X$, $\Omega = 1/2$) and (D, $\Omega = 1/2 - X$, $\Omega = 1/2$) transitions of KrF* and XeF* and a weak broad (C, $\Omega = 3/2 - A$, $\Omega = 3/2$) transition of KrF* were identified by reference to reported data [3,4,19]. In the longer wavelength region of fig. 3b, a similar weak broad (C, $\Omega = 3/2$ -A, $\Omega = 3/2$) transition of XeF* extended up to ≈ 550 nm. Outstanding features of the KrF* and XeF* emissions in comparison with those from the reactions of $Kr({}^{3}P_{2})$ and $Xe({}^{3}P_{2})$ with fluorine-containing molecules [3,4] are that oscillatory structure is either weak or absent for all the observed transitions. This is probably due to low-vibrational excitation in the emitting states.

The only rare gas active species which are gener-



Fig. 3. KrF* and XeF* emissions produced from ion recombination between (a) Kr⁺ and SF₆⁻ (He: 1.6 Torr; Kr: 15 mTorr; SF₆; 15 mTorr) and (b) Xe⁺ and SF₆⁻ (He: 0.65 Torr; Xe: 10 mTorr; SF₆; 15 mTorr) in the He afterglow. The optical resolution is 2.9 Å (fwhm).

ated by He(2³S)/Kr and He(2³S)/Xe Penning ionization are Kr⁺ and Xe⁺ in the ground ${}^{2}P_{3/2,1/2}$ states [18]. The Kr⁺/SF₆ and Xe⁺/SF₆ reactions cannot be responsible for the KrF^{*} and XeF^{*} excimer formation based upon the energetics. It was, therefore, concluded that the KrF^{*} and XeF^{*} emissions arise from ion-neutralization processes:

$$Kr^{+} + SF_{6}^{-} \rightarrow KrF^{*}(B, C, D) + SF_{5},$$
 (9)

$$Xe^{+}+SF_{6}^{-} \rightarrow XeF^{*}(B, C, D)+SF_{5}.$$
 (10)

The observation of RgF* excimer emissions due to dissociative ion recombination is consistent with the kinetic study of KrF* and XeF* by Cooper et al. [16] in pulse radiolysis. However, the present finding contradicts the result of Wren et al. [15] who predicted that process (10) is closed. On the basis of the present finding, dissociative ion recombination (10) must play an important role in their tesla-discharge experiment of Xe/SF₆ mixtures, where significant quantities of both Xe⁺ and electrons were present. The XeF* spectrum obtained in the tesla discharge

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is quite similar to that from process (10), supporting the above conclusion.

The excimer formation by reactions of $Rg^*({}^{3}P_{0,2})$ with halogen-containing molecules has been extensively studied by Setser and co-workers using the FA method [1-11]. According to their results the fraction of available energy deposited into RgX^* excimer is relatively small for molecules which form stable parent RX^- negative ions. The unimolecular decay of a long-lived $[Rg^+RX^-]$ complex dominates the energy disposal. The low-vibrational excitation of RgF^* observed here for SF_6 , which produces stable SF_6^- ions, probably reflects such mechanism.

Emission spectra of SF₆ in the Ar and Kr afterglows were observed by introducing a small amount of SF₆ from the first gas inlet. No excimer emission was detected at low rare gas pressures (≤ 0.15 Torr for Ar and ≤ 50 mTorr for Kr) where Ar(${}^{3}P_{0,2}$) and $Kr({}^{3}P_{2})$ were energy carriers. This observation is consistent with the previous FA result of Velazco et al. [3]. At higher rare gas pressures (≥ 0.2 Torr for Ar and >60 mTorr Kr) where ionic active species were involved in the discharge flow, ArF* and KrF* emissions were observed as shown in fig. 4. When ionic active species were removed from the discharge flow by using the ion-collector grid, all excimer bands disappeared completely. This shows that ionic species are responsible for the excimer formation. Possible ionic active species are Ar+, $(Ar^+)^*$, Kr^+ , and $(Kr^+)^*$: the presence of the former two ions were confirmed by monitoring the $OCS^+(A-X)$ emission from Ar^+/OCS [24] and the CH(A-X) emission from $(Ar^+)^*/CH_4$ [25]. The spectral features of the observed ArF* and KrF* emissions are very similar to those obtained from processes (9) and (10) except that the D-X transition of KrF* is very weak. It was, therefore, reasonable to assume that the ArF* and KrF* emissions result from the same processes. The Ar⁺ and Kr⁺ ions are dominantly produced in the microwave discharge of Ar and Kr. Electrons which attach to SF₆ to form SF_{6}^{-} are probably generated by the following excitation transfer reactions:

$$(Ar^+)^* + SF_6 \rightarrow SF_n^+ (n = 3-6)$$

+ $(F_2 \text{ and/or } F) + Ar^+ + e^-$, (11)



Fig. 4. ArF* and KrF* emissions produced from ion recombination between (a) Ar* and SF₆⁻ in the Ar afterglow (Ar: 0.4 Torr; SF₆: 5 mTorr) and (b) Kr⁺ and SF₆⁻ in the Kr afterglow (Kr: 62 mTorr; SF₆: 12 mTorr). The optical resolution is 2.9 Å (fwhm) for (a) and 4.7 Å for (b).

$$(Kr^+)^* + SF_6 \rightarrow SF_n^+ (n=5-6) + (F) + Kr^+ + e^-,$$
(12)

where $(Ar^+)^*$ and $(Kr^+)^*$ stand for metastable ions with available energies of 16.4–20.3 and 14.9–16.3 eV, respectively [26], for excitation transfer such as processes (11) and (12).

The most outstanding feature of the KrF* emission from the Kr^+/SF_6^- reaction in the Kr afterglow is that the relative intensity of D-X to B-X and C-A is very weak. Since SF₆ was added to the Kr afterglow ≈ 15 cm downstream from the center of the discharge, most of the $Kr^+({}^2P_{1/2})$ ions is expected to be de-excited to the ground ${}^{2}P_{3/2}$ spin-orbit state by collisions with Kr atoms and by superelastic collisions with electrons as found in the $Ar^+({}^{2}P_{1/2,3/2})$ ions [27]. On the other hand, the ${}^{2}P_{1/2}/{}^{2}P_{3/2}$ ratio produced from Penning ionization (3) is expected to be much larger at a short distance between the Kr and SF₆ inlets (≈ 1 cm). The D-X/B-X ratio depended upon the distance between the Kr and SF₆ inlets and the SF₆ pressure. When Kr was admitted to the He flow from the first gas inlet and then SF₆ was added from the third gas inlet placed 10 cm downstream from the second one (not shown in fig. 1), the D-X/B-X ratio became very weak because of the collisional de-excitation from ${}^{2}P_{1/2}$ to ${}^{2}P_{3/2}$. The spectral appearance was similar to that obtained in the Kr afterglow. On the contrary, the D-X band was enhanced with increasing the SF_6 pressure, because the quenching rate constant of ${}^{2}P_{3/2}$ by SF₆ is larger than that of ${}^{2}P_{1/2}$ by about one order of magnitude [28]. The measurements of the KrF* emission at various ${}^{2}P_{1/2}/{}^{2}P_{3/2}$ ratios lead us to conclude that the B and C states are preferentially formed through the Kr⁺ ($^{2}P_{3/2}$) reaction, while Kr⁺ ($^{2}P_{1/2}$) favors the D state. The state selectivity can be explained by the diabatic potential diagram shown in fig. 5. According to the diagram, dissociative recombination proceeds through diabatic pathways predicted from the potential diagram. The present finding is consistent with the relative formation constants of the RgX*(B, C, D) states by the metastable Ar* and Kr* atoms in the ${}^{3}P_{0,2}$ spin-orbit states in which a propensity for conservation of the Rg⁺ ion-core configuration was found [10,11]; the ${}^{3}P_{2}$ atoms form the B and C states through an $[Rg^+({}^2P_{3/2})RX^-]$ ion



Fig. 5. Schematic potential energy diagram for $[Rg^+({}^{2}P_{3/2,1/2})SF_{6}]$ and RgF^* states obtained from refs. [15,19]. It is assumed that SF_{6}^+ dissociates into $F^- + SF_{5}$ in the presence of Rg^+ and ion-pair $[Rg^+F^-]$ intermediates are formed. The broken lines over the entrance channels represent the quasi-continuum of SF_{6}^* excited states.

pair, whereas the ${}^{3}P_{0}$ atoms yield the D state through an $[Rg^{+}({}^{2}P_{1/2})RX^{-}]$ ion pair.

A similar significant enhancement of D-X relative to B-X is found for the XeF* excimer obtained from process (10) in comparison with that from the reactions of Xe(${}^{3}P_{2}$) with fluorine-containing molecules [3]. This is probably due to the fact that the D state is produced through the direct Xe⁺(${}^{2}P_{1/2}$)/ SF₆⁻ reaction in the present experiment, whereas a core switching from Xe⁺(${}^{2}P_{3/2}$) to Xe⁺(${}^{2}P_{1/2}$) is required at the crossing between the covalent and ionic surfaces for the formation of the D state in the Xe(${}^{3}P_{2}$) reaction. Since the D-X transition of ArF* was located outside the present observation region, it was difficult to obtain information on the state selectivity of process (8).

There are quasicontinuous Rg+RX* (excited states) product channels below the $V(Rg^+, RX^-)$ potential for a relatively large molecule such as SF_6 (see fig. 5). In addition, a number of Rg**(Rydberg states) + RX potentials are present above the $Rg^*(metastable states) + RX$ potential, though they are not shown in fig. 5 for the sake of clarity. If the attractive ion-pair potential strongly couples with some of these $V(Rg, SF_6^*)$ or $V(Rg^{**}, SF_6)$ potentials, this coupling diverts trajectories from the ionpair potential to the $V(Rg, SF_6^*)$ or $V(Rg^{**}, SF_6)$ potentials. The observation of strong RgF* emissions from the $Rg^+ + SF_6^-$ reactions suggests that such a coupling is weak, so that the ion-pair potential can pass through the large number of the $V(Rg, SF_6^*)$ and $V(Rg^{**}, SF_6)$ potentials.

It is of interest to consider why excimer formation channels are closed for the $Rg^*({}^{3}P_{0,2})/SF_6$ reactions. Since Penning ionization is energetically inaccessible in the energy transfer reactions of $Ar({}^{3}P_2)$, $Kr({}^{3}P_2)$, and $Xe({}^{3}P_2)$ with SF_6 , the formation of SF_6^* , probably followed by dissociation or predissociation into fragments, must be the dominant exit channels. Curve-crossing models for energy transfer from Rg^* to SF_6 require crossing of potential surfaces correlating with Rg^*+SF_6 (or $Rg^++SF_6^-$ if charge transfer occurs) and the product $Rg+SF_6^*$ surfaces. If charge-transfer intermediates are involved in the reaction, the cross section can be estimated from the relation

$$\sigma_{\rm CT} = \pi R_{\rm c}^2 \,, \tag{13}$$

where R_c is the Rg-SF₆ separation at the crossing point. R_c is given by

$$R_{\rm c} = e^2 / (\rm{IP} - \rm{EA}) ,$$
 (14)

where IP is the ionization potential of Rg* and EA is the electron affinity of SF_6 [29]. By using an EA value of ≈ 0.5 eV [30], σ_{CT} is calculated to be ≈ 47 , ≈ 47 , ≈ 51 , and ≈ 59 Å² for Ar(³P₂), Ar(³P₀), $Kr({}^{3}P_{2})$, and $Xe({}^{3}P_{2})$, respectively. These values are comparable to the total quenching cross sections of 36, 38, 51 and 75 Å² for Ar(${}^{3}P_{2}$), Ar(${}^{3}P_{0}$), Kr(${}^{3}P_{2}$), and $Xe({}^{3}P_{2})$, respectively [5]. It is therefore possible that charge-transfer intermediates participate in the SF^{*}₆ formation. The intermediate stages of the Rg* reaction pathways, which proceed via an ion-pair intermediate, closely resemble the dissociative recombination processes (8)-(10). The difference is that (8)-(10) have higher, $IP(Rg) - E(Rg^{*}, {}^{3}P_{0,2})$, available energies. Perhaps [Rg+SF₆] complex predissociates efficiently into Rg+SF^{*}₆ in the Rg^{*} reactions, whereas the additional energy of Rg⁺, relative to Rg*, results in the RgF* formation before the intermediate complex predissociates. There is an alternative explanation to the absence of excimer formation in the Rg*/SF6 reactions that does not depend on the RgF* formation from the ion-pair intermediate. The efficiency of transfer from $V(Rg^*,$ SF_6) to $V(Rg^+, SF_6^-)$ may be small for such a large molecule as SF₆. Quenching then would take place by direct transfer from $V(Rg^*, SF_6)$ to $V(Rg, SF_6^*)$ at short range. Further detailed experimental and theoretical studies are necessary to determine the relative importance of the two explanations.

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