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ARTICLE *in* CHEMICAL PHYSICS LETTERS · MAY 1999

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## A new excited electronic state of SF<sub>2</sub> radical observed by resonance-enhanced multiphoton ionization

Quanxin Li, Qun Zhang, Jinian Shu, Shuqin Yu, Qinhua Song, Congxiang Chen,  
Xingxiao Ma \*

*Department of Chemical Physics, University of Science and Technology of China (Key Laboratory for Bond-Selective Chemistry, Chinese Academy of Sciences), Hefei, Anhui 230026, PR China*

Received 5 August 1998; in final form 22 March 1999

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### Abstract

The resonance-enhanced multiphoton ionization (REMPI) spectrum of SF<sub>2</sub> radical has been recorded between 235 and 270 nm. A pulsed dc discharge technique was applied to generate neutral SF<sub>2</sub> radicals. Analyses of the laser intensity index and vibrational progression indicate that the spectrum arises from one-photon resonance between the ground-state  $\tilde{X}^1A_1$  and a previously unobserved  $\tilde{B}'$  state. The band origin and vibrational frequency  $\omega'_1(a_1, \text{sym.}, \text{str.})$  were determined as 38 623 and  $926 \pm 4 \text{ cm}^{-1}$ , respectively. The  $\tilde{B}'$  state seems to be a valence state with relatively strong predissociation for  $v' \geq 3$  levels. © 1999 Elsevier Science B.V. All rights reserved.

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### 1. Introduction

There is considerable interest in SF<sub>2</sub> radical because of its potential importance in semi-conductor manufacturing. It has been proved that SF<sub>2</sub> radicals play a significant role in plasma etching by SF<sub>6</sub>/O<sub>2</sub> [1–4]. Previously, many efforts have been made to study the ground state of the SF<sub>2</sub> radical and its cation [5–10]. However, the spectroscopic and structural information on the excited electronic states of the neutral SF<sub>2</sub> radical was relatively limited. Glinski et al. observed an emission spectrum from 550 to 860 nm in the gas-phase reaction of F<sub>2</sub> with CS<sub>2</sub>, and first assigned it to be from the FCS radical [11], but reassigned it to the transition of the SF<sub>2</sub>( $\tilde{A} \rightarrow \tilde{X}$ ) system afterwards [12]. The electronic origin of  $\tilde{A}^1B_1$

lies near  $18\,500 \pm 1200 \text{ cm}^{-1}$ . The  $\tilde{B}(4s)$  and the  $\tilde{E}(4p)$  Rydberg states of the SF<sub>2</sub> radical have been identified by the pioneering REMPI work of Johnson and Hudgens [13]. The band origins and the vibrational frequencies of the 4s and 4p Rydberg states have been derived from this work. A valence state  $\tilde{C}$  which overlaps the vibrational progression of the 4s Rydberg state between  $57\,000$  and  $60\,000 \text{ cm}^{-1}$  was also observed [13]. More recently, we have investigated the electronic band systems of SF<sub>2</sub> radical between  $54\,945$  and  $81\,630 \text{ cm}^{-1}$  by  $(2 + 1)$  REMPI spectroscopy [14]. The  $\tilde{F}$  state with  $\nu_{0-0}$  of  $63\,812 \text{ cm}^{-1}$  which merges with the vibrational progression of the  $\tilde{E}(4p)$  state was identified. The four higher Rydberg states,  $\tilde{G}(3d_1)$ ,  $\tilde{H}(3d_2)$ ,  $\tilde{I}(3d_3)$  and  $\tilde{J}(5s)$ , respectively, were also observed [14]. Moreover, some theoretical investigations have been made to identify the equilibrium geometries, excitation ener-

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\* Corresponding author. E-mail: xxma@ustc.edu.cn

gies, force constants and vibrational frequencies of the ground state and several excited electronic states for SF<sub>2</sub> radical [15–24] [25,26].

In this Letter we use a dc electric discharge to produce the neutral SF<sub>2</sub> radicals. A new excited electronic state  $\tilde{B}'$  whose energy lies between the  $\tilde{A}$  and  $\tilde{B}(4s)$  states, was revealed by one-photon resonance-enhanced multiphoton ionization spectroscopy between 237 and 270 nm. In order to identify the REMPI mechanism, measurement of the REMPI ion signal as a function of laser intensity and analysis of the vibrational structure were carried out. The related spectral constants of the  $\tilde{B}'$  state have been derived.

## 2. Experimental

The experimental apparatus has been described in detail elsewhere [14]. It consists of a pulsed radical generation source, a pulsed Nd:YAG-pumped frequency-doubled dye laser, a time-of-flight mass spectrometer, and a computer data acquisition system.

SF<sub>2</sub> radicals were produced by pulsed dc discharge in a pulsed molecular beam of Ar seeded with SF<sub>6</sub> (30%). In order to produce a stable discharge in the pulsed beam, a special design was used. The pulsed dc discharge was conducted between a pair of copper electrodes with four closely spaced pairs of tungsten needles. Then a stable glow discharge was created between a pair of parallel copper plates. The background ions produced by the discharge were effectively eliminated by two reflectors, which consisted of three skimmers, all with the same diameter of 1 mm.

The light source used was a dye laser (Lumonics: HT500) pumped with the Nd:YAG laser (Spectra Physics: GCR-170). The dye laser output was then doubled by a frequency-doubler (Lumonics: HT1000). The frequency-doubled dye laser (energy 0.02–2.6 mJ/pulse; bandwidth  $\sim 0.08$  cm<sup>-1</sup>) directly entered into the center of the photoionization zone through a small hole ( $\varnothing \approx 2$  mm). The dye laser wavelength was calibrated against known neon and argon atomic transitions using optogalvanic spectroscopy [27,28]. The ion-current signals from the time-of-flight mass spectrometer were amplified, recorded, and averaged. The relative time-delays

among the nozzle, the dc discharge, and the laser were controlled by a pulsed multi-channel delay generator.

The gas samples used were SF<sub>6</sub> (99.99%) and argon (99.999%). The entire experimental apparatus and method used for the present REMPI studies of free radical have proved reliable by carefully observing the known spectra of SO, CH<sub>3</sub>, and CF radicals, which were produced by the pulsed dc discharge of SOCl<sub>2</sub>/Ar, CH<sub>3</sub>I/Ar, and CF<sub>4</sub>/Ar mixtures, respectively.

## 3. Results and discussion

SF<sub>2</sub> radicals were generated by the pulsed dc discharge in the mixtures of SF<sub>6</sub> and argon. As shown in Fig. 1, three typical mass spectra were measured under the following conditions: (a) dc discharge alone; (b) 258.91 nm laser irradiation alone; and (c) dc discharge together with 258.91 nm laser irradiation. The strong  $^{32}\text{SF}_2^+$  ( $m/z = 70$ ) ion signal appeared only in case (c), which reflected that the SF<sub>2</sub><sup>+</sup> should be attributed to neither the discharge ions nor the MPI products of parent molecules (SF<sub>6</sub>). In order to further identify the spectral carrier, we have observed the (2 + 1) REMPI spectra between 290 and 360 nm by using the present discharge technique. The observed vibrational progressions associated with the 4s and 4p Rydberg states agreed quite well with the previous observation by Johnson and Hudgens [13]. In addition, the vibrational analysis on the  $\tilde{B}'$  state (see below) also supported that the spectral carriers were the neutral SF<sub>2</sub> radicals.

Fig. 2 shows the mass-selected REMPI spectrum of the SF<sub>2</sub> radical between 235 and 270 nm under a 'soft' ionization condition (using a low-power unfocused laser beam). Over the wavelength range of this measurement the ion signal was only carried by the ion  $^{32}\text{SF}_2^+$  ( $m/z = 70$ ). The REMPI spectrum shown in Fig. 2 displays one prominent progression of five regularly spaced vibrational bands. Along the progression the average *one-photon energy interval* between band maxima is  $\sim 926$  cm<sup>-1</sup>. Compared with the vibrational frequencies of  $\omega'_1(a_1, \text{sys.}, \text{str.})$  of  $991 \pm 12$  cm<sup>-1</sup> for the 4s Rydberg state and  $\omega'_1(a_1, \text{sys.}, \text{str.})$  of  $931 \pm 59$  cm<sup>-1</sup> for the 4p Rydberg state [13], the interval of 926 cm<sup>-1</sup> is believed

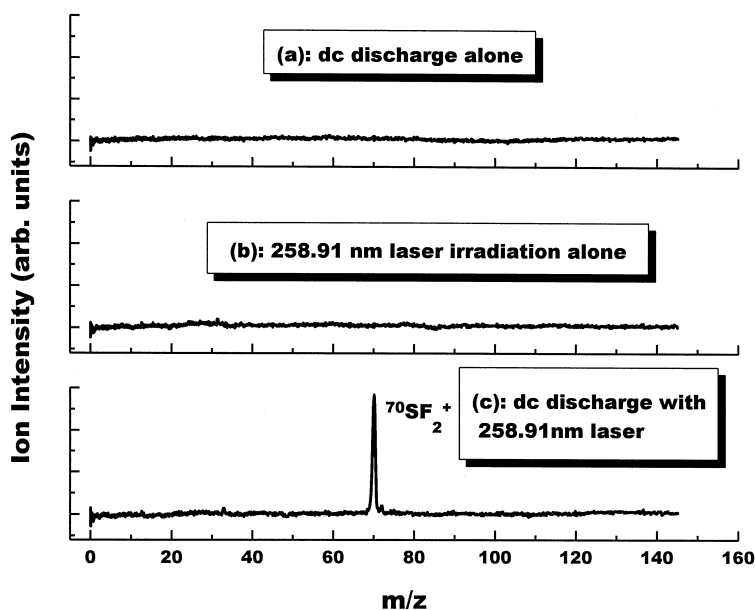


Fig. 1. Three typical mass spectra under: (a) the dc discharge alone; (b) the 258.91 nm laser irradiation alone; and (c) the dc discharge together with the 258.91 nm laser irradiation. The  $^{32}\text{SF}_2^+$  ( $m/z$  70) ion signals appeared only in the case (c).

to be the  $\omega'_1$  vibrational frequency of an excited electronic state of the  $\text{SF}_2$  radical. Therefore the observed REMPI spectrum should arise from a one-photon resonance.

In order to further examine the multiphoton ionization mechanism, the intensity of the  $\text{SF}_2^+$  ions was measured as a function of the laser intensity (see Fig. 3). The laser energy was monitored from 20  $\mu\text{J}$  to 2.6 mJ. The cross-sectional area of an unfocused UV laser beam was estimated as 0.03  $\text{cm}^2$ , resulting in a photon flux of  $(0.01\text{--}1) \times 10^{25}$   $\text{photon cm}^{-2} \text{s}^{-1}$  [29]. As shown in Fig. 3, the plot of  $\log I_{\text{ion}}$  against  $\log I_{\text{laser}}$  is very close to a linear relationship. A small deviation from the line seems to appear for laser intensities lower than  $3 \times 10^{23}$   $\text{photon cm}^{-2} \text{s}^{-1}$ . The derived slope of the solid line in Fig. 3 was  $\sim 0.67$ . The part of the curve below  $3 \times 10^{23}$   $\text{photon cm}^{-2} \text{s}^{-1}$  appears to have a slope closer to 1. This results can be explained as showing a linear dependence for one-photon absorption at lower power with some saturation at higher photon flux. The adiabatic ionization potential  $\text{IP}_a$  of 10.08 eV ( $81\,301 \text{ cm}^{-1}$ ) for the  $\text{SF}_2$  radical has been measured by the potential energy surface (PES) [30]. Energetically, a  $\text{SF}_2$  radical in the ground state must absorb three photons

to ionize and form the ground-state cation for wavelengths longer than 246 nm. Thus, the REMPI spectrum for the first three vibrational bands should be from a  $(1+1+1)$  or a  $(1+2)$  MPI process. It is noted that the probability of a direct two-photon transition is  $\rho = \sigma I^2 \Delta t \approx 10^{-9}$  under the present experimental condition (typical cross-section for two-photon absorption  $\sigma \approx 10^{-51} \text{ cm}^4 \text{ s}$  [31],  $I_{\text{laser}} \approx 10^{25} \text{ photon cm}^{-2} \text{ s}^{-1}$  and  $\Delta t \approx 10^{-8} \text{ s}$ ). This

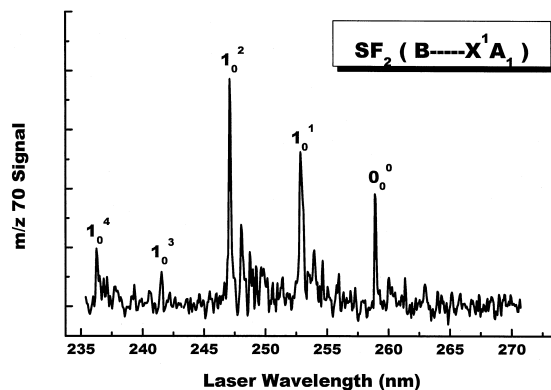


Fig. 2. REMPI spectrum of  $^{32}\text{SF}_2$  ( $m/z$  70) radical observed between 235 and 270 nm.

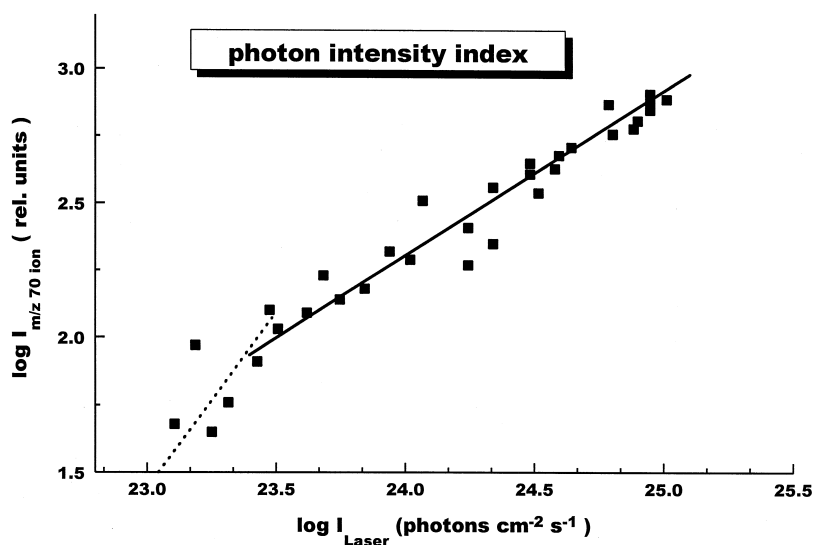


Fig. 3. Typical double-logarithmic dependence of the  $^{32}\text{SF}_2^+$  ( $m/z = 70$ ) REMPI ion signals measured as a function of laser intensity at 247.10 nm.

implies that a direct two-photon transition should not be saturated. In addition, the measured photon index was  $n \leq 1$ . Therefore, the most likely REMPI steps between 246 and 270 nm may be as follows:  $\text{SF}_2(\text{X})$  radical absorbs one photon to excite to an electronic state, then ionizes after absorbing another two single photons one by one, i.e., a  $(1 + 1 + 1)$  multiphoton ionization mechanism for the first three vibrational bands. Since the ionization requires only two-photon energy between 235 and 246 nm, the overall ionization should occur through a  $(1 + 1)$  REMPI step for the vibrational bands of 241.55 and 236.25 nm. The  $\text{SF}_2^+$  ions formed would be the ground-state ions,

since the first electronically excited state of the  $\text{SF}_2^+$  ( $\tilde{\text{A}}^2\text{A}_1$ ) is  $\sim 5.32$  eV higher than the ground-state  $\text{SF}_2^+$  ( $\tilde{\text{X}}^2\text{B}_1$ ). Thus, we believe that the REMPI spectrum between 235 and 270 nm is associated with the transition from the ground state to an excited electronic state of the  $\text{SF}_2$  radical (labeled as  $\tilde{\text{B}}'$  state).

Table 1 lists the band positions, assignments, one-photon energy, and band intervals of the observed progression, the difference between the two-photon energies and the first ionization potential, and the possible mechanisms. Based upon the above analyses, we assigned the progression to the activity

Table 1

Band positions, assignments, spacings observed in the REMPI spectrum of  $^{32}\text{SF}_2$  radical between 235 and 270 nm, differences between the two-photon energies and the ionization potential ( $2h\nu - \text{IP}_a$ )<sup>a</sup>, and possible mechanisms

Assign.	Band pos., $\lambda_{\text{air}}$ (nm)	State energy ( $\text{cm}^{-1}$ )	Energy rel. to $\tilde{\text{B}}'(0_0^0)$ ( $\text{cm}^{-1}$ )	$\omega_1$ band interval ( $\text{cm}^{-1}$ )	$2h\nu - \text{IP}_a$ ( $\text{cm}^{-1}$ )	Mechanism
$\tilde{\text{B}}' 0_0^0$	258.91	38623	0		−4054.1	1 + 1 + 1
$\tilde{\text{B}}' 1_0^1$	252.85	39549	926	926	−2202.7	1 + 1 + 1
$\tilde{\text{B}}' 1_0^2$	247.10	40469	1846	920	362.1	1 + 1 + 1
$\tilde{\text{B}}' 1_0^3$	241.55	41399	2776	930	1497.6	1 + 1
$\tilde{\text{B}}' 1_0^4$	236.25	42328	3705	929	3355.1	1 + 1
				$\bar{\omega}_1 = 926 \pm 4 \text{ cm}^{-1}$		

<sup>a</sup>The ionization potential of  $81301 \text{ cm}^{-1}$  is from Ref. [30].

of the  $\omega'_1(a_1, \text{sys.}, \text{str.})$  mode for the  $\tilde{B}'$  state. The vibrational frequencies  $\omega'_1(a_1, \text{sys.}, \text{str.})$  of  $926 \pm 4 \text{ cm}^{-1}$  can be yielded. The terminus at  $258.91 \text{ nm}$  ( $h\nu = 38\,623 \text{ cm}^{-1}$ ) in the vibrational progression is assigned as the electronic band origin of the  $\tilde{B}'$  state. No other resonance was detected in the wavelength range longer than  $260 \text{ nm}$  under the present experimental conditions.

We had expected that the  $\tilde{B}'$  state is a Rydberg state of the  $\text{SF}_2$  radical since the observed vibrational frequency  $\omega'_1 = 926 \pm 4 \text{ cm}^{-1}$  is similar to those values of the  $4s$  and  $4p$  Rydberg states [13]. In general, quantum defect ( $\delta$ ) of a Rydberg state may vary only within a limited range for each orbital type [32,33]. For sulfur-centered Rydberg orbitals, the  $\delta$  values of the  $ns$ ,  $np$ ,  $nd$  and  $nf$  Rydberg states should lie near  $2.0$ ,  $1.6$ ,  $0.08$  and  $0.06$  [34], respectively. Quantum defects can be derived by the familiar Rydberg formula:

$$\nu_{0-0} (\text{cm}^{-1}) = \text{IP}_a - 109737/(n - \delta)^2,$$

where  $\nu_{0-0}$  is the electronic state origin,  $\text{IP}_a$  the adiabatic ionization potential in  $\text{cm}^{-1}$ ,  $n$  the principal quantum number, and  $\delta$  the quantum defect. Using the assigned origin for the  $\tilde{B}'$  state and the adiabatic ionization  $\text{IP}_a = 81\,301 \text{ cm}^{-1}$  [30] for  $\text{SF}_2$  to solve the Rydberg equation, we yield the values of  $n = 3$  and  $\delta = 1.4$ . The  $\delta$  value seems too small for the  $np$ -type Rydberg state [34]. Alternatively, the electronic origin of the  $3p$  Rydberg state appears near  $25\,500 \text{ cm}^{-1}$  estimated by  $\delta_{3p} = 1.6$ . But the observed origin of the  $\tilde{B}'$  state is near  $38\,623 \text{ cm}^{-1}$ . Therefore, we think that the  $\tilde{B}'$  state might not be a  $3p$  Rydberg state. Fig. 2 also displays that the intensities of the vibrational bands for  $v' \geq 3$  decrease heavily. These variations of the intensities do not arise from the change of the laser power, and may reflect the predissociation of vibrational levels for  $v' \geq 3$ .

The occupied molecular orbital of the ground state for the  $\text{SF}_2$  radical are described in  $\text{C}_{2v}$  symmetry group by the configuration:

$$1a_1^2 2a_1^2 1b_2^2 3a_1^2 1b_1^2 4a_1^2 2b_2^2 5a_1^2 3b_2^2 6a_1^2 2b_1^2 7a_1^2 4b_2^2 \\ 1a_2^2 5b_2^2 8a_1^2 3b_1^2.$$

The lowest-lying valence state  $\tilde{A}^1 B_1$  ( $\nu_{0-0} \approx 18\,500 \text{ cm}^{-1}$ ) was observed by the previous emission spec-

trum [12], which arises from the promotion of an electron from the HOMO  $3b_1$  orbital to the LUMO  $9a_1$  orbital. The calculated excitation energies [25,26] for  $\tilde{X}^1 A_1 \rightarrow \tilde{A}^1 B_1$  are in good agreement with experimental data [12]. The  $\tilde{B}^1 A_1$  state investigated by the  $(2+1)$  REMPI spectra [13,14] is a  $4s$  Rydberg state which forms from the excitation of the  $3b_1$  into the diffuse Rydberg orbital with the configuration (in  $\text{C}_{2v}$ ):  $\dots 5b_2^2 8a_1^2 3b_1^2 4sa_1^1$ . The higher valence state  $\tilde{C}$  was also observed between  $56\,219$  and  $61\,278 \text{ cm}^{-1}$  by  $(2+1)$  REMPI spectra [13,14]. This state possesses the orbital configuration:  $\dots 5b_2^2 8a_1^1 3b_1^2 6b_2^1$  with symmetry of  $\tilde{C}^1 B_2$  by theoretical prediction [26]. To the best of our knowledge, no excited electronic states were observed between the  $\tilde{A}$  state and the  $\tilde{B}(4s)$  Rydberg state. The  $\tilde{B}'$  state investigated by the present  $(1+1+1)$  or  $(1+1)$  REMPI spectrum lies between  $38\,623$  and  $42\,328 \text{ cm}^{-1}$ . Although the equilibrium geometries and excitation energies for several excited electronic states of the  $\text{SF}_2$  radical have been investigated theoretically [15–24] [25,26]. Unfortunately, no theoretical calculations corresponding to the excitation energy of  $\sim 38\,623$ – $42\,328 \text{ cm}^{-1}$  were investigated. Obviously, both experimental and theoretical studies are needed to further clarify the features (e.g., the orbital configuration, the symmetry and the life time, etc.) for the  $\tilde{B}'$  state of the  $\text{SF}_2$  radical.

#### 4. Conclusions

A pulsed dc discharge technique was used to generate the neutral  $\text{SF}_2$  radical in a molecular beam of  $\text{Ar}/\text{SF}_6$ . The REMPI spectrum corresponding to  $^{32}\text{SF}_2^+$  ( $m/z = 70$ ) was investigated in the excitation wavelength range of  $235$ – $270 \text{ nm}$ . According to the analyses of the observed spectrum and the photon intensity index, the REMPI spectrum was assigned as a one-photon resonance between the ground state and a new electronic state  $\tilde{B}'$ . The spectroscopic constants of the  $\tilde{B}'$  state for  $\text{SF}_2$  were obtained.

#### Acknowledgements

We would like to thank National Natural Foundation of China, the State Education Commission and

National 95-Climbing Project of China for financial support. We also thank Mr. Lin Hongfa and Mr. Gao Hui for their assistance during the construction of the experimental apparatus.

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