Angular Correlation Between B K-VV Auger Electrons of BF_3 Molecules and Coincident Fragment Ions: Manifestation of the Difference Between the Angular Correlation and Molecular Frame Auger Electron Angular Distribution

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We have measured the angular correlation between the B K-VV Auger electrons of BF_3 molecules and the coincident fragment-ion pairs of $BF_2{}^+$-F^+. Then, we have found that the measured angular correlation patterns depending on the mutual angle between the light polarization direction and molecular orientation are affected by the anisotropic axis distribution of the molecular ensemble of $BF_3{}^+$ reflecting the anisotropic nature of photon-molecule interaction. In this context, we have pointed out generally that for coincidence experiments, so-called molecular frame Auger electron angular distributions are realized only if the axis distribution of the molecular ion ensemble is isotropic.

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Most of the experimental and theoretical studies of molecular Auger processes have concentrated on determining the energy and probability of a given Auger transition [1–7]. Additional information can be obtained when Auger electrons are distinguished by their direction of emission. Relevant theories for molecules in the gas phase were developed by several authors [8–10]. Finally, the most informative is the study of the Auger electron angular distribution (AEAD) ejected from fixed-in-space molecules. Reflecting this, Auger processes of fixed-in-space diatomic molecules have been theoretically considered [11–15]. In these theories, the Auger processes are described by a two-step approximation, in which two amplitudes of inner-shell photoionization and subsequent Auger decay appear as a simple product [16]. The two-step formula can be derived from a general one-step formula by simply neglecting the exchange effects between two electrons due to their large energy difference. Then, the two-step model is justified when energies of the photoelectron and Auger electron are largely different. Even so, when the photon energy is close to the threshold of inner-shell ionization, the subsequent Auger decay may be influenced by the presence of the slowly receding photoelectron, which can shield the doubly charged ion. The resulting interaction between the escaping electrons is called a postcollision interaction (PCI) [16,17], which causes a breakdown of the two-step model. However, at high photon energies the PCI effect gives negligible influence. Thus, under the above-mentioned circumstances the two-step model gives a reliable formula of AEAD from fixed-in-space molecules as follows [12–15]:

$$\frac{d\sigma}{d\hat{\mathbf{k}}_{\mathrm{ion}}d\hat{\mathbf{k}}'_A} \simeq [1+\beta_{\mathrm{ion}}P_2(\cos\theta_{\mathrm{ion}})] \times\left[\sum_K(-1)^K(2K+1)\alpha_K^A P_K(\cos\theta'_A)\right], \qquad (1)$$

where $\hat{\mathbf{k}}_{\mathrm{ion}}=(\theta_{\mathrm{ion}},\phi_{\mathrm{ion}})$ is the fragment ion direction in the laboratory coordinate frame (LF), z axis along the electric field vector of the incident light, $\hat{\mathbf{k}}'_A=(\theta'_A,\phi'_A)$ is the Auger electron momentum direction in the molecular coordinate frame (MF), β_{ion} is the asymmetry parameter for the fragment ions, α_K^A is expressed by the Coulomb matrix elements describing the Auger decay, and P_K is the Kth Legendre polynomial. Here the axial recoil approximation, in which the fragment-ion direction coincides with the molecular z axis at the moment of the inner-shell photoionization, is used. The second factor of Eq. (1) is described in MF, so that it is often called molecular frame AEAD (MF-AEAD), it is independent of the photoionization process. However, it should be emphasized that in general obtainable data using the electron–fragment-ion coincidence technique are not the MF-AEAD, but the angular correlation between the Auger electrons and fragment ions which are detected in LF. Such angular correlation is necessarily affected by the anisotropic axis-distribution of the molecular ion ensemble described by $\beta_{\mathrm{ion}}\neq 0$, the first factor of Eq. (1). Only if the axis distribution is fully isotropic, $\beta_{\mathrm{ion}}=0$, the angular correlation function reduces to the MF-AEAD. Unlike this, in the experiments of Refs. [18–20] the axis distribution is not isotropic. Nevertheless, the authors of the literature have reported that the angular correlations are not dependent on the light polarization, but only on the molecular axis. On the contrary, the angular correlations depending on both the photon energy and light polarization have been demonstrated in Ref. [21]. This long-standing controversial problem is really puzzling. It is the purpose of the present work to shed light on the puzzling problem with careful measurements of the angular correlations and with the correct interpretation of it. Recently the most sophisticated measurements of the angular correlation, in which Auger final states are resolved by selecting kinetic energy release of fragment-ion pairs, have been reported in Refs. [22–25]. However, from these results one cannot judge whether the observed angular correlation is dependent on the polarization or not, because the measurements have been performed for a specific light polarization geometry relative to the fragment-ion direction.

In this Letter, we report the experimental results on the angular correlations between the B K-VV Auger electrons of BF_3 molecules and their coincident ion pairs of BF_2^+-F^+ under various light polarization geometries. To understand the experimental results qualitatively, we have applied the general formula of the angular correlation function [14] derived within the framework of the two-step and axial-recoil approximation and neglecting possible influences of PCI. In the formula, the effect of the orbital angular momentum coupling between the Auger electrons and fragment ions is explicitly described through the β_{ion} for fragment ions. Until now, such effect has been overlooked, although every experiment has been performed by coincidence measurements between the Auger electrons and fragment ions.

The experiment was carried out at the undulator beam line BL-2C of the 2.5 GeV storage ring at the Photon Factory. The experimental method and velocity map imaging apparatus were described elsewhere [26], so that only a brief outline is given. Linearly polarized soft x rays from a planar undulator were monochromatized using a varied-space plane grating monochromator [27,28] and focused onto a supersonic molecular beam of BF_3, where the photon beam crossed perpendicularly to the molecular beam. The axis of the velocity map imaging spectrometer was aligned to the y axis, which is perpendicular to the coplanar x-z plane defined by the photon propagation direction and the polarization vector. Photoelectrons and fragment ions were extracted into opposite directions along the y axis by an electrostatic field, and were detected by position-sensitive detectors (PSDs) consisting of microchannel plates and delay-line anodes, which were placed parallel to the x-z plane. The momentum vectors of fragment ions were deduced from positions (x_{ion}, z_{ion}) on the PSD and flight times of these products. The projection of the electron momentum vectors on the coplanar x-z plane was determined from positions (x_e, z_e) on the PSD. The triple coincidence signals of the two-body fragment ion pairs of BF_2^+-F^+ and B K-VV Auger electrons (or B 1s photoelectrons) were analyzed to obtain the vector correlations between them on the coplanar x-z plane. Thus, we determined the following observables from one set of measurements: the asymmetry parameter β_e for the B 1s photoelectrons, β_A for the B K-VV Auger electrons, β_{ion} for the fragment ion pair, the B 1s photoelectron angular distribution in the recoil frame (RF) of BF_2^+-F^+, and the angular correlation between the B K-VV Auger electrons and coincident ion pairs of BF_2^+-F^+ in LF. Note that the angular correlation between the photoelectrons and coincident ion pairs of BF_2^+-F^+ is equivalent to the photoelectron angular distribution in RF under the axial recoil approximation, because the ensemble of molecules BF_3 is randomly oriented. This situation is realized for resonance Auger electron emission from the inner-shell excited state of randomly oriented molecules, as well. To obtain polar angle distributions of electrons we integrated photoelectron (Auger electron) signals over ±5° (±10°) in the coplanar x-z plane, and ±25° (± 30°) perpendicular to the plane. On the fragment ion we integrated the signals over ±10° in the coplanar x-z plane, and ±25° perpendicular to that plane.

Figure 1(a) shows the two dimensional momentum image of electrons, and Fig. 1(b) demonstrates the momentum image of the fragment ion pair of BF_2^+-F^+. These images were measured at the photon energy of 263 eV. From the data of the B 1s photoelectrons with 60 eV energy [see also Fig. 1(c)] in LF, we have determined $\beta_e = 1.20 \pm 0.03$. Further, from the data the B K-VV Auger electrons with ~150 eV energy [see also Fig. 1(c)] in LF, we have determined $\beta_A = -0.025 \pm 0.010$. Besides these, the momentum image of the fragment ion pair with the kinetic energy release ≥ 9 eV [see Fig. 1(d)] gives the information on the axis distribution of the molecular ion BF_3^+ at the instant of the B 1s ionization,

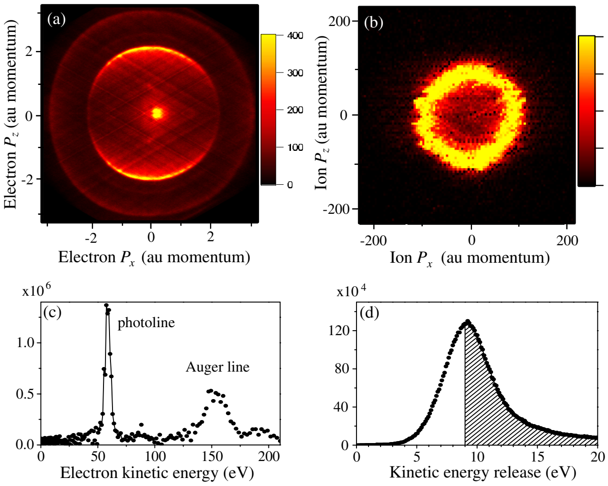

FIG. 1 (color online). (a) Two-dimensional electron momentum distributions with polarization along the z axis. (b) Two-dimensional ion momentum distributions. (c) Electron energy spectrum obtained by peeling the electron momentum distributions in (a). (d) Kinetic energy release spectrum of the fragment ion pair of BF_2^+-F^+. An outer ring, an inner ring, and a central bright part in (a) is due to the B K-VV Auger electrons, the B 1s photoelectrons, and shake-off electrons, respectively.

$\beta_{\rm ion} = -0.036 \pm 0.021$. This value of the asymmetry parameter is consistent with the result, $\beta_{\rm ion} = -0.062$, of our time dependent density functional theory (TDDFT) calculations [29], which deviates from the $\beta_{\rm ion} = 0$ predicted from the statistical weight of the optical allowed transitions of $2a_1'(\mathrm{B}1s) \rightarrow e'$ (parallel component to the molecular plane) and $2a_1'(\mathrm{B}1s) \rightarrow a_2''$ (perpendicular component to the molecular plane). Namely, above the $2a_1' \rightarrow e'$ shape resonance the TDDFT calculations exhibit a weak modulation of the $2a_1' \rightarrow e'$ ionization cross section due to photoelectron diffraction by the neighboring F atoms. The modulation has the minimum at the photon energy of 243 eV. As a result of this, $\beta_{\rm ion} = -0.25$ at the minimum. It is marked that the modulation of the cross section causes the anisotropic axis distribution of the molecular ions, $\beta_{\rm ion} = -0.062$ even at the photon energy of 263 eV.

Before considering our main subject, we discuss the B 1s photoelectron angular distribution in RF of $\mathrm{BF_2}^+$-F^+. The B 1s photoelectron angular distribution in RF (z axis along the recoil direction) is shown in Fig. 2 together with the results of TDDFT calculations. Because the experiment does not detect the orientation of the fragment ion of $\mathrm{BF_2}^+$ about the recoil direction, the measured photoelectron angular distribution necessarily includes an average of it in MF over the azimuthal angle about the recoil direction. After this average, we obtain an expression similar to the linear molecule case [30,31]. In the comparison of the experimental data with the theoretical, one can see that there are some differences on the lobe and node structures of the angular distributions. However, one can recognize from Fig. 2 that the main node position of the theoretical results, which is caused by the symmetry restriction of the continuum wave function and then sensitive to the recoil direction, coincides with the node of the experimental data for the different polarization geometry in Figs. 2(a)–2(d). As a consequence of this, it is allowed that the axial-recoil approximation is valid within the experimental accuracy. Therefore, we neglect the rotational motion of the molecule, and assume undoubtedly that the fragment-ion pair of $\mathrm{BF_2}^+$-F^+ recoils back-to-back along the B-F bond.

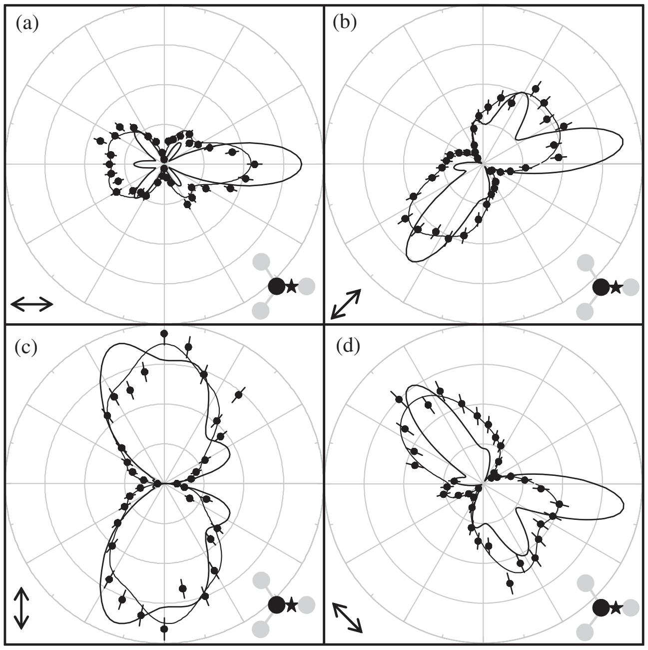

FIG. 2. B 1s photoelectron angular distribution in the recoil frame of $\mathrm{BF_2}^+$-F^+. Closed circles with error bars: experimental data. Solid lines: TDDFT calculations. The experimental data are normalized to the calculated by the integrated area. Double headed arrows indicate the polarization vector. A star on a molecular model represents the bond-breaking position of the two-body fragmentation of $\mathrm{BF_2}^+$-F^+. The $2a_1' \rightarrow e'$ and $2a_1' \rightarrow a_2''$ transitions are involved in (b), (c), and (d). In (a), only the $2a_1' \rightarrow e'$ transition contributes.

We will consider our main subject. Let $\hat{\mathbf{k}}_A = (\theta_A, \phi_A)$ be the direction of the Auger electron momentum and $\hat{\mathbf{k}}_{\rm ion} = (\theta_{\rm ion}, \phi_{\rm ion})$ the direction of the F^+ ion of the fragment-ion pair in LF. Transforming the $\hat{\mathbf{k}}_A' = (\theta_A', \phi_A')$ in MF of Eq. (1) into $\hat{\mathbf{k}}_A = (\theta_A, \phi_A)$ in LF and dropping the restriction to the particular direction $\hat{\mathbf{k}}_{\rm ion} = (\theta_{\rm ion}, \phi_{\rm ion})$, the angular correlation function in LF is obtained as follows [14]:

$$W(\theta_A, \phi_A; \theta_{\rm ion}, \phi_{\rm ion})|^{\text{2-step}}_{\text{lin.pol.}} = \sum_{KL\mu} A^{KL}_{\mu}(h\nu) Y_{K\mu}(\theta_A, \phi_A) Y^*_{L\mu}(\theta_{\rm ion}, \phi_{\rm ion}). \qquad (2)$$

Here, $Y_{\kappa\mu}(\hat{\mathbf{k}})$ are the spherical harmonics and A^{KL}_{μ} are dynamical parameters of the process given by

$$A^{KL}_{\mu}(h\nu) = (-1)^K \alpha^A_K 4\pi \Big[\delta_{KL} + \beta_{\rm ion}\sqrt{\frac{2K+1}{2L+1}} \times (20K-\mu|L-\mu)(20K0|L0) \Big], \qquad (3)$$

where δ_{KL} is the Kronecker symbol and Clebsch-Gordan coefficients are employed. K and L are the vector sum of orbital angular momentum of the Auger electron and fragment ion, respectively. The Auger decay parameter α^A_K consists of the absolute square of the Coulomb matrix element $\langle f; \ell m | V_c | i \rangle$ in terms of partial wave expansion of the Auger electron wave function $|\mathbf{k}_A\rangle$. Strictly, the expansion is done by the symmetry-adapted spherical harmonics [9], but here it is abbreviated by (ℓm) for brevity. Note that the α^A_0 is normalized to unity. Equation (3) shows the direct connection between the orbital angular momentum coupling and $\beta_{\rm ion}$, i.e., the anisotropic axis distribution of the molecular ion ensemble following the photoionization. A necessary condition for the existence of the Coulomb integral is that the direct product $\Gamma(f) \times \Gamma(\ell m)$ must contain the irreducible representation (IR) of A_1', because $\Gamma(i) = A_1'$. Here, $\Gamma(i)$, $\Gamma(\ell m)$ and $\Gamma(f)$ are the IR of the initial state of $\mathrm{BF_3}^+$, $|\mathbf{k}_A\rangle$ and the final state of $\mathrm{BF_3}^{2+}$, respectively. Although the final states with all the possible IR belonging to the D_{3h} point group are assigned in the preceding works [32,33], individual Auger lines are not resolved in the present work. Then, we discuss the angular correlation in an average of all the Auger lines involved in the band pass of our spectrometer [see Fig. 1(c)]. The observed angular correlation for different geometries is shown in Figs. 3(a)–3(d). It should be noticed that the angular correlation pattern becomes cylindrically symmetric relative to the polarization direction only for the geometry in Fig. 3(a). As a natural consequence of this, one can see in the figures that the angular correlation pattern depends on the mutual angle between the fragment-ion pair and polarization direction. If one fixes the recoil direction of the fragment-ion pair like in Figs. 3(a)–3(d), one can say that the angular correlation pattern depends on the polarization direction. This does not mean a breakdown of the two-step approximation at all, because Eq. (2) is derived within the two-step model. In other words, whether the angular correlation is dependent on the polarization or not is irrelevant to the validity of the two-step model, although it has been used for checking the validity in the previous works [18–21]. The angular correlation depending on the polarization comes from the anisotropy of the axis distribution of the molecular ion ensemble, i.e., $\beta_{\rm ion} = -0.036 \pm 0.021$. The second term of Eq. (3) contributes to the angular correlation pattern in the different manner via specific values $Y^*_{L\mu}(0°, 0°)$, $Y^*_{L\mu}(45°, 0°)$, $Y^*_{L\mu}(90°, 0°)$, and $Y^*_{L\mu}(135°, 0°)$ of the spherical harmonics. If the axis distribution of the molecular ion ensemble is isotropic, i.e., $\beta_{\rm ion} = 0$, then the contribution of the second term of Eq. (3) disappears. In this special case, the angular correlation pattern becomes independent of the light polarization, in other words, it reduces to the MF-AEAD. On the other hand, in the more general case of $\beta_{\rm ion} \neq 0$, one might say roughly that the value of $\beta_{\rm ion}$ indicates the extent of the contribution of the second term of Eq. (3) in the angular correlation pattern. In the present results for the different geometries, one can see the intensity variation of the angular correlation pattern within the range of about ±10% of the mean intensity in Figs. 3(a)–3(d), which is consistent with our value of $\beta_{\rm ion} = -0.036 \pm 0.021$. In this connection, the self-consistency of our present data can be evaluated as follows. Integrating the angular correlation data over all the fragment-ion pair directions, we have obtained the AEAD from randomly oriented molecular ions in LF, i.e., as can be derived from Eqs. (2) and (3) $\beta_{\rm ion}\alpha^A_2 = \beta_A$. That is, we have determined $\beta_{\rm ion}\alpha^A_2 = -0.020 \pm 0.014$. This value is close to $\beta_A = -0.025 \pm 0.010$ for the AEAD in LF. This ensures the self-consistency of our present data. The structure of the angular correlation pattern shown in Fig. 3 might be due to the contributions of the higher orbital angular momenta of the Auger electrons.

We briefly argue the previous results. The angular correlation between the C K-VV Auger electrons of CO molecules and their fragment ions is displayed by polar plots on a plane in Fig. 3 of Ref. [21], although the Auger electrons and fragment ions were detected in different planes. It is supposed that to get the polar plots the authors have transformed the Auger electron momentum into a plane including fragment-ion momentum. However, such transformation seems to be unlikely without the information on the azimuthal angle dependence of the AEAD. Then we cannot understand what their data at 299 and 305 eV mean. When $\beta_{\rm ion} = 0$ and the angular correlation reduces to MF-AEAD, the transformation gives meaningful results. In fact, their angular correlation data at the photon energy of 400 eV look like the MF-AEAD being independent of the polarization, reflecting the small value of $\beta_{\rm ion} = 0 \pm 0.05$ at that energy. Later, the authors of Ref. [18] appealed that the angular correlation patterns of the same process as Ref. [21] at 305 eV do not depend on the polarization, see Fig. 3 of Ref. [18]. However, one notices the angular correlation patterns are not the same for the different polarization, especially for the circular polarization. A more serious problem is that the angular correlation patterns of Refs. [18,21] are completely differentt. The most probable reason for the strong discrepancy may be due to the inaccurate transformation in Ref. [21]. In both Ref. [19] for CO and Ref. [20] for N_2, the authors calculated the MF-AEADs with the use of Eq. (1), that is, dividing their measured angular correlation data by the first factor of Eq. (1). This procedure is inadequate, as discussed above. But, we can examine their angular correlation data. They exhibit the polarization dependence in accord with our interpretation; see Fig. 3 of Ref. [19] and Fig. 2 of

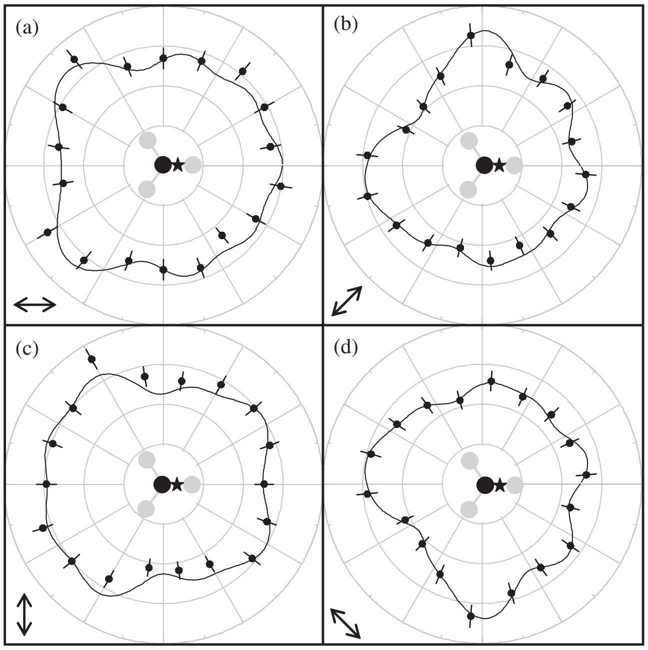

FIG. 3. Angular correlation between the B K-VV Auger electrons and fragment ion pairs of $BF_2{}^+$-F^+. Closed circles with error bars: experimental data. The full curves are drawn for guide the eye. Double headed arrows indicate the polarization vector. A star on a molecular model represents the bond breaking position of the two-body fragmentation of $BF_2{}^+$-F^+. The direction of the two-body fragmentation defines the molecular orientation at the instant of B 1s photoionizaton.

Ref. [20]. Moreover, the angular correlation data at 500 eV in Ref. [20] are almost independent of the polarization, due to the small value of β_{ion} at that energy.

In conclusion, we have revealed that the angular correlation depending on the mutual angle between the polarization and fragment-ion pair direction is controlled by the anisotropy parameter β_{ion} describing the axis distribution of the molecular ion ensemble. This interpretation has resolved the long-standing controversial problem on the angular correlation data [18–21]. Although we have discussed the angular correlation on an average of individual B K-VV Auger transitions, the present discussion is applicable to each Auger line, which will exhibit a richly structured angular correlation pattern. It should be mentioned that the very recent work reports the AEAD for each N K-VV Auger transition from laser aligned N_2 molecules, which exhibits characteristic features due to the symmetries of the Auger final states [34]. The AEAD from such prealigned molecules is the MF-AEAD, because the molecular axes of them are pointing one and the same direction. More importantly, our present results on the angular correlation are quite general phenomena, so that they provide a new basic understanding on the Auger decay of the molecular system, and are essentially important not only for molecular physics, but also for a wider range of science involving surfaces, clusters, solid states, and biomolecules.

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