Kinetic energy release in the dissociations of doubly and triply charged molecular ions

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A system for 3D recoil-ion momentum spectroscopy (RIMS) [1] was used to measure the spectra of kinetic energy release (KER) in the dissociations of doubly and triply charged ions of CO, N_2, and O_2 molecules produced by bombardment of neutral molecules with 2.5 MeV/u Xe^{34+} projectiles. Similar results are expected for any collision system in which $Q_p / v_p >> 1$ and $v_p >> 1$, where Q_p is the projectile charge and v_p is the projectile speed relative to the molecule, expressed in atomic units. Negligible dependence on the projectile species and energy in this collision regime is a result of the fact that for large values of Q_p / v_p the projectile interacts with the target at large average (or most probable) impact parameter b. If Q_p / v_p is increased, b increases as well, so that $Q_p / v_p\ b$ remains nearly constant and the net effect of the Coulomb interaction remains unchanged. Additionally, at large impact parameters, other available ionization mechanisms (such as single and multiple electron capture) can be neglected compared to direct Coulomb ionization (DI).

Figure 1 shows (by the thin red lines) the KER spectra obtained in the present work for the following reactions:

(A) $CO^{2+} \rightarrow C^+ + O^+$,

(B) $N_2^{2+} \rightarrow N^+ + N^+$,

(C) $O_2^{2+} \rightarrow O^+ + O^+$,

(D) $CO^{3+} \rightarrow C^{2+} + O^+$,

(E) $N_2^{3+} \rightarrow N^{2+} + N^+$, and

(F) $O_2^{3+} \rightarrow O^{2+} + O^+$.

Also shown in Figure 1 are the corresponding best-available KER spectra obtained by other authors under similar conditions (i.e., in the strong interaction regime with fast heavy ion projectiles and measured by means of RIMS). Such results are very scarce; virtually limited to just two groups. A survey of the available results is presented in Table I. Evidently, KER spectra for dissociations C, D, and F have not been presented previously.

The KER FWHM resolution of the present system was assessed by a propagation of errors procedure applied to each event based on the measured resolution of the molecular-fragments' times of flight and that of their impact positions on the detector. The results obtained for the dissociations (A) and (D) are shown in Figure 2. It is evident that the KER FWHM resolution has a distribution that depends on the KER value. Furthermore, it was found that all of these distributions are effectively bounded by lines representing a direct proportionality between the minimum or maximum KER FWHM resolution and the square root of the corresponding KER (see the black lines in Figure 2). The constants of proportionality (in $eV^{1/2}$) were found to be 0.106 and 0.198 for dissociation (A) and 0.130 and 0.342 for dissociation (D). Therefore, in the region between the peaks in the KER spectra [6 - 20 eV for (A) and 19 - 30 eV for (D)] the KER FWHM resolution ranges between 0.26 eV and 0.88 eV and between 0.56 eV and 1.9 eV, respectively. However, it should be noted that most of the events in the peaks have KER

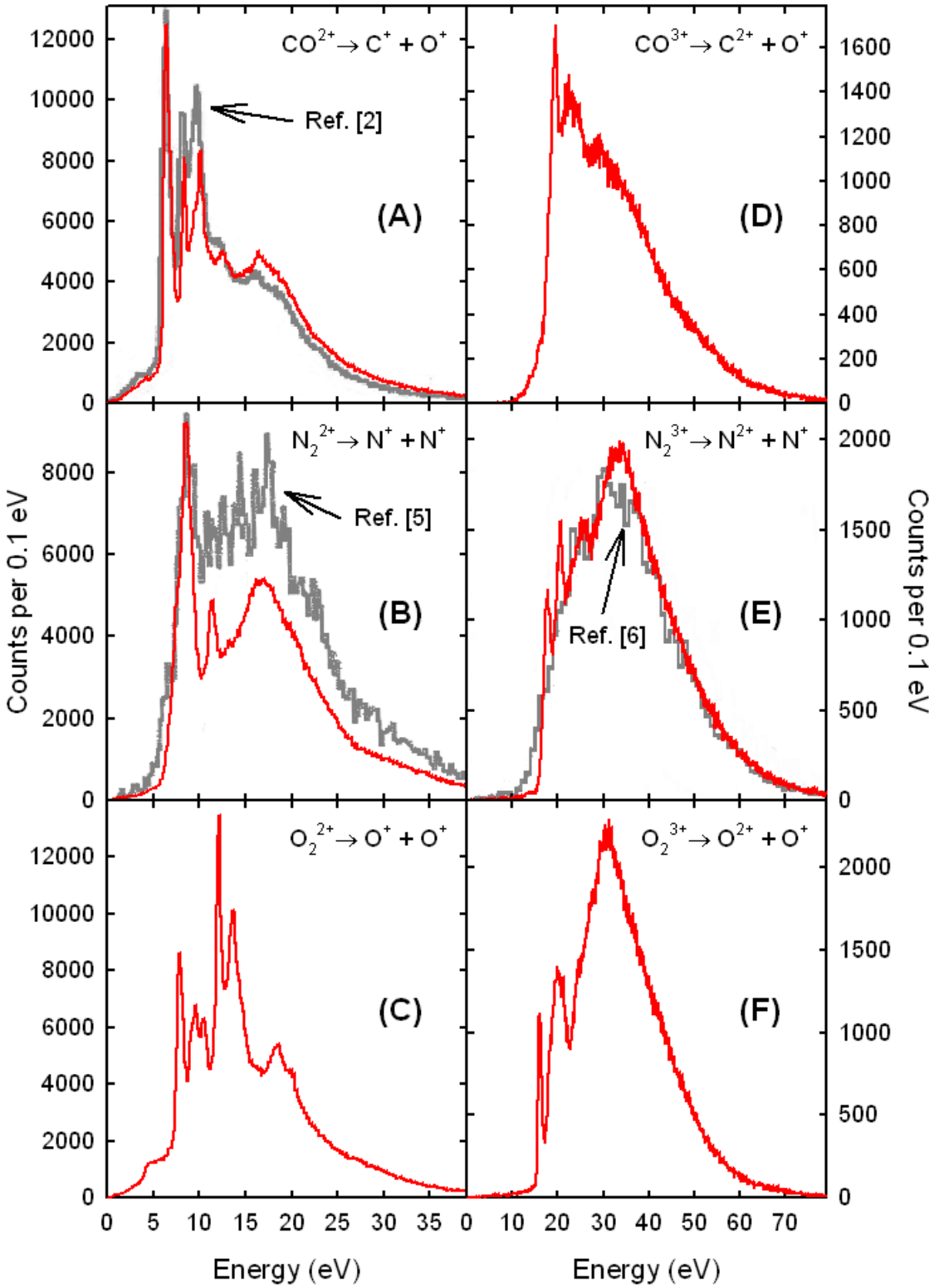

FIG. 1. Total kinetic energy release (KER) spectra for the dissociations (A) $CO^{2+} \rightarrow C^+ + O^+$, (B) $N_2^{2+} \rightarrow N^+ + N^+$, (C) $O_2^{2+} \rightarrow O^+ + O^+$, (D) $CO^{3+} \rightarrow C^{2+} + O^+$, (E) $N_2^{3+} \rightarrow N^{2+} + N^+$, and (F) $O_2^{3+} \rightarrow O^{2+} + O^+$. Spectra obtained in the present work are shown by the red lines, while the best-available spectra obtained previously by other authors under similar conditions (as specified in the text) are shown by the gray lines.

Table I. Survey of the available KER spectra for the dissociation of doubly and triply charged ions of CO, N_2 and O_2 molecules, measured in the strong collision regime by means of recoil-ion momentum spectroscopy.

Beam energy (MeV/u)	Beam Species	Beam Charge State	Projectile speed Vp(au)	Somerfeld parameter Qp/vp	Target	KER spectra shown	Ref.
8.0	Ni	24+	18	1.3	CO	C^+O^+	[2]
3.6	Xe	21+	12	1.7	CO	C^+O^+	[3]
2.5	Xe	34+	10	3.4	CO	C^+O^+, $C^{2+}O^+$	Present
5.9	Xe	17+	15	1.1	N_2	N^+N^+	[4]
5.9	Xe	43+	15	2.8	N_2	N^+N^+	[5]
4.7	Bi	26+	14	1.9	N_2	N^+N^+	[5]
4.7	Bi	57+	14	4.2	N_2	N^+N^+	[5]
3.6	Xe	40+	12	3.3	N_2	N^+N^+, $N^{2+}N^+$	[6]
2.5	Xe	34+	10	3.4	N_2	N^+N^+, $N^{2+}N^+$	Present
5.9	Xe	18+	15	1.2	O_2	n/a*	[7]
5.9	Xe	43+	15	2.8	O_2	n/a*	[7]
2.5	Xe	34+	10	3.4	O_2	O^+O^+, $O^{2+}O^+$	Present

*See the text

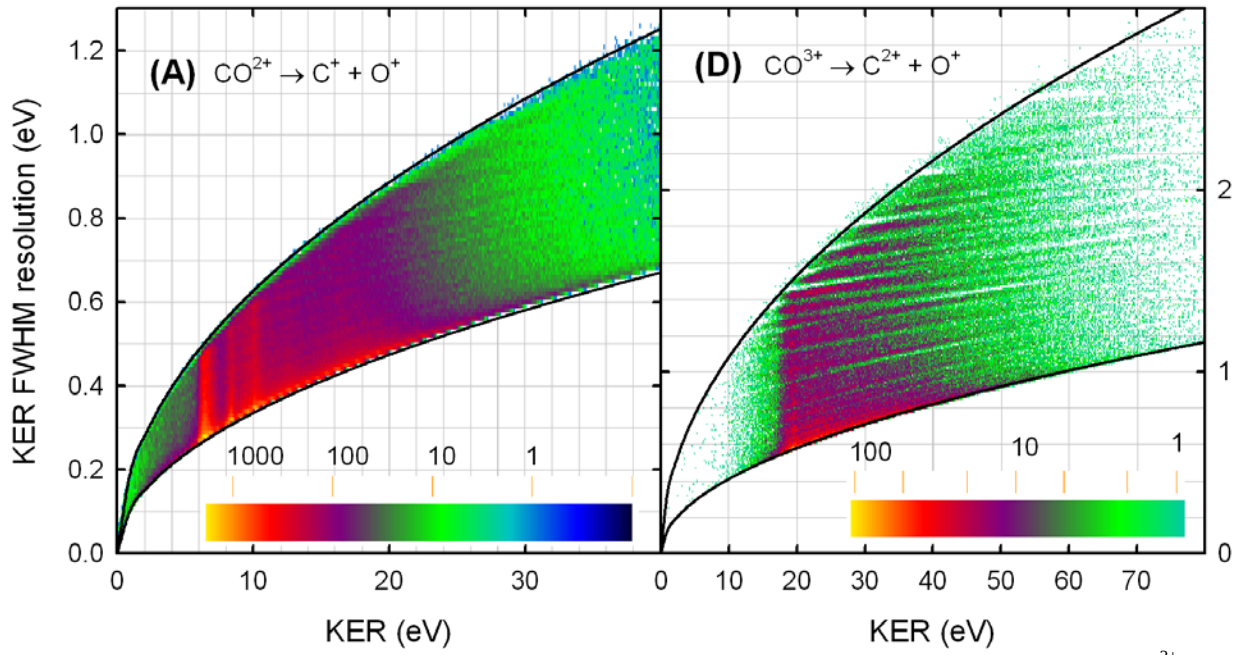

FIG. 2. Two-dimensional histograms of KER FWHM resolution versus KER for the dissociations (A) $CO^{2+} \rightarrow C^+ + O^+$ and (D) $CO^{3+} \rightarrow C^{2+} + O^+$. The boundaries delineated by the black lines represent upper and lower limits that are described in the text.

FWHM closer to the lower limit. This is especially true for the peak at 6.4 eV in Figure 1 (A), for which

the lower limit of the KER FWHM resolution is about 0.26 eV. This resolution is comparable to or better than that obtained in the previously published measurements under similar conditions.

For dissociation (B), Figure 1 (B) compares the present KER spectrum with a spectrum obtained using 5.9 MeV/u Xe^{43+} projectiles [5]. While the KER resolution of the two spectra seems comparable, the rather poor statistics of the spectrum from Ref. 5 does not allow for a detailed comparison. It is noticeable, though, that the high-energy side of the spectrum from Ref. 5 displays significantly higher intensity relative to the low-energy peak.

For dissociation (E), Figure 1 (E) compares the present KER spectrum with the only available KER spectrum measured by other authors under similar conditions. The latter spectrum was obtained using 3.6 MeV/u Xe^{40+} projectiles [6]. Apparently, the KER resolution of Ref. 6 was too poor to observe the triple peak structure displayed by the present data. Other than that, the overall shape of the spectrum appears to be essentially the same.

As noted above, no other published spectra obtained under similar conditions were found for dissociations (C), (D) and (F). However, such measurements were reported for dissociations (C) and (F) [7], but it was stated that no significant structure was observed. The energies of peak channels observed in the KER spectra for dissociations (D), (E), and (F) in the present work are given in Table II.

Table II. Energies (eV) of peak channels in the present KER spectra for the dissociation of triply charged ions of CO, N_2 and O_2 molecules.

Reaction	Peak channel energy (eV)
$CO^{3+} \rightarrow C^{2+} + O^{+}$	19.5
	22.5
	29.4
$N_2^{3+} \rightarrow N^{2+} + N^{+}$	17.8
	20.7
	25.2
	24.5
$O_2^{3+} \rightarrow O^{2+} + O^{+}$	15.9
	19.8
	31.2

The spectra shown in Figure 1 (D-F) are believed to be the best available at the present time. A detailed analysis of these spectra will require extensive calculations of the potential energy curves for the parent molecular ions.

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