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# Inner-shell photodetachment from the $K^-$ ion

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**Abstract**
We have measured the relative cross section for photodetachment from the $K^-$ ion for the process $K^- + h\nu \rightarrow K^+ + 2e^-$ over the photon energy range 21–24.5 eV. The structures in the measured cross section are associated with correlated processes involving the detachment or excitation of a 3p core electron, processes which are often accompanied by the excitation of one or more valence electrons. The most prominent feature in the cross section is a strong resonance arising from the excitation of a 3p electron from the core and a 4s valence electron. As in previous experiments on double excitation of valence electrons, electron correlation is seen to play an important role in the dynamics of negative ions.

Negative ions are structurally different from atoms and positive ions due primarily to the enhancement of the effect of the correlated motion of the electrons arising from the efficient screening of the nucleus by the atomic electrons. Electron correlation often dominates the structure and dynamics of these weakly bound systems. Accurate measurements of the properties of negative ions provide sensitive tests of the ability of theory to go beyond the independent-electron model. We describe in the present paper an experimental study of the excitation and detachment of electrons from the $K^-$ ion following the absorption of a photon in the vacuum ultraviolet region (VUV) of the electromagnetic spectrum. The focus of the paper is an investigation of resonances associated with the production and decay of doubly excited states of $K^-$ ions in which a 3p core electron and a 4s valence electron are simultaneously excited. The present study of the $K^-$ ion complements a previous investigation of similar resonances in $Na^-$ [1].

Until relatively recently, photodetachment studies of negative ions have concentrated on the ejection of valence shell electrons [2–6]. In these studies it is often found that the cross sections are modulated by the presence of resonance structure. Such resonances are associated with the excitation and subsequent autodetaching decay of a doubly excited state of the ion, in which two valence electrons are simultaneously excited. These studies are primarily laser based. The advent of high-brightness synchrotron radiation sources that produce UV and x-ray photons has made it possible to extend such studies to inner shell electron detachment [1, 7–11].

The $K^-$ ion has a ground state that is dominated by the configuration $3p^64s^2$. In this and other configuration labels used in this paper, the inert $1s^22s^22p^63s^2$ core is omitted. The binding energy of the $3p^64s^2\ {}^1S$ ground state of $K^-$ is numerically equal to the electron affinity of the K atom, which has been measured to be 0.501 459(12) eV [12]. The potential well associated with the short-range binding force in the case of the $K^-$ ion supports only one bound state. There is, however, a rich spectrum of excited states involving either the excitation of a pair of valence electrons or a core electron and a valence electron. Core-vacancy excited states of $K^-$ in the energy range of the present study, ∼20–25 eV, are expected to have dominant configurations of the type $3p^54sn\ell n'\ell'$ in which a 3p core and a 4s valence electron are simultaneously excited. These states will decay by autodetachment since they are embedded in $3p^54sn\ell + e^-$ continua associated with core detachment from the K atom. Continua such as these have structure in the form of core-vacancy excited states of K with configurations of the type $3p^54s^2$, $3p^53d4s$, $3p^54s5s$, $3p^54d4s$, $3p^54s5d$. Pegg *et al* [13] observed such states in K in a study of collisions between $K^+$ and He gas. The observed spectrum of Auger electrons was produced in the decay of core-vacancy excited states of K. The energies of many core-vacancy states of atoms can be found in the literature [14]. The tabulated energies of these states in the K atom are useful in identifying the corresponding states of the $K^-$ ion observed in the present experiment, since the configurations of the latter typically differ from those of the former by just a single weakly bound spectator electron. This makes it possible to estimate the energies of core-vacancy excited states of $K^-$ by adding the electron affinity of K to the listed energies of the corresponding core-vacancy states of K. The core-vacancy excited states $K^-$ ($3p^54sn\ell n'\ell'$) have odd parity since they connect via E1 radiation to the even parity $K^-$ ($3p^64s^2$) ground state. The $K^-$ ion has a ground-state symmetry of ${}^1S$, and so the excited states must have a ${}^1P^o$ symmetry. This implies that the two outermost electrons, $n\ell$ and $n'\ell'$ must both have orbital angular momentum quantum numbers, $\ell$ and $\ell'$, that are even. The intermediate core-vacancy states $3p^54sn\ell$ ($\ell = 0,2$) of K that are formed in the autodetachment of the doubly excited ${}^1P^o$ states of $K^-$ are restricted by the selection rules on Coulomb autodetachment to states of ${}^2P^o$ and ${}^2D^o$ symmetry. Many such states with configurations of the type $3p^54s^2$, $3p^53d4s$, $3p^54s5s$, $3p^53d5s$, $3p^54d4s$, $3p^54s5d$, $3p^54s6s$ and $3p^54s6d$ lie in the energy range 18.7–24.0 eV, relative to the ground state of the K atom [14]. Generally speaking, core-vacancy excited states of the $K^-$ ion are weakly bound relative to the corresponding states of the K atom and manifest themselves as Feshbach resonances in the photodetachment cross section.

The autodetachment of a core-vacancy excited state of $K^-$ produces a core-vacancy state of K, which, in turn, decays preferentially via the Auger process to form a $K^+$ ion. Since radiative decay is highly improbable in the case of the core-vacancy states of K, the detected $K^+$ ions can be used as a reliable monitor of the cross section for photodetachment from $K^-$. The partial energy level diagrams for $K^-$, K and $K^+$ that are shown in figure 1 indicate

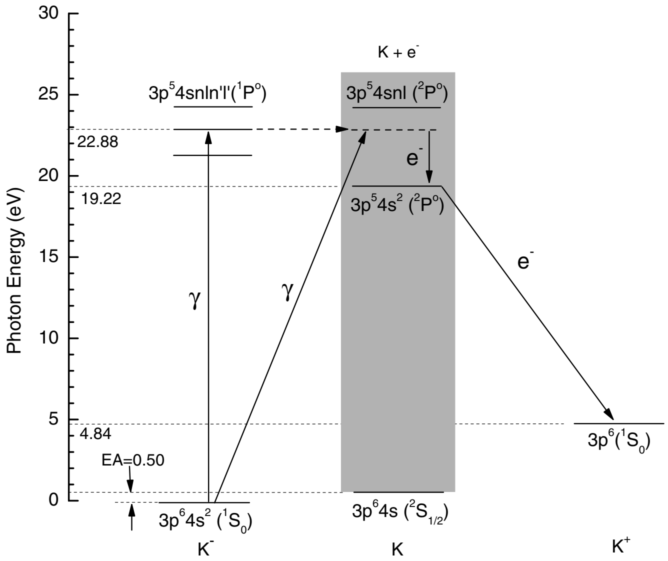


**Figure 1.** A partial energy level diagram for K$^-$, K and K$^+$ systems. The relevant photoexcitation ($\gamma$) and electron emission (e$^-$) processes are shown.

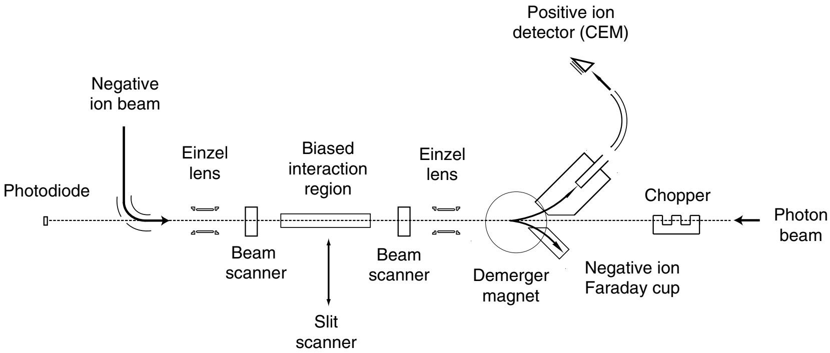


**Figure 2.** Schematic diagram of photon-negative ion merged beams apparatus

the energy range in which one would expect to find core-excited states of K$^-$ involving the simultaneous excitation of a 3p and 4s electron.

The experiment was performed at the 10.0.1 undulator beam line using the 10.0.1.2 photon–ion-beam endstation at the advanced light source (ALS) situated at the Lawrence Berkeley National Laboratory. The merged-beams apparatus used in the present experiment is shown in figure 2. It has been described in detail in a previous publication [15]. The photon beam from the synchrotron source was collinearly overlapped with a beam of K$^-$ ions from a low-energy accelerator equipped with a negative ion sputter source. The K$^-$ ions were extracted from the ion source at 5 keV and focused using a series of cylindrical electrostatic lenses. The ion beam was then momentum selected using a 60° analysing magnet. The transverse area of the ion beam was defined by two sets of adjustable slits mounted in a plane perpendicular to the direction of motion of the ion beam. After the ion beam was momentum selected and collimated, it was merged onto the axis of a counter-propagating beam of photons from the synchrotron source using a set of 90° spherical-sector bending plates. The primary ion beam then entered a 29.4 cm long cylindrical interaction region which was biased at +2 kV to energy label the $K^+$ ions as a result of the photon–ion interaction. This energy-labelling process enabled us to localize the region from which we detect $K^+$ ions.This, in turn, allowed us to maximize the signal associated with $K^+$ ions produced by the absorption of a photon and minimize the signal from $K^+$ ions produced in double-detachment collisions of the $K^-$ ions with the residual gas in the unbiased region of the ion-beam line. This background contribution was further minimized by maintaining a vacuum pressure of $5 \times 10^{-10}$ Torr in the beam line. The spatial overlap of the ion and photon beams was measured in the centre of the interaction region using a stepping-motor-driven slit scanner. Rotating-wire profile monitors were used just upstream and downstream of the interaction region to ensure that the two beams were well collimated over the entire interaction region. Fine tuning of the overlap of the two beams was achieved by using two sets of perpendicular electrostatic steering plates mounted immediately behind the spherical sector plates used to merge the ion beam onto the axis of the photon beam.

After the interaction region, a 45° analysing magnet was used to separate the energy-labelled $K^+$ ions produced in the biased interaction region from the primary $K^-$ beam. These $K^+$ ions had an energy of 9 keV, whereas the collisionally detached $K^+$ background ions produced in the beam line external to the interaction region had an energy of 5 keV, as determined by the extraction voltage at the ion source. The small background consisting of 9 keV $K^+$ ions produced by collisional detachment in the interaction region was measured and accounted for by chopping the photon beam at a frequency of 6 Hz. The $K^+$ ions were further deflected, out of the vertical dispersion plane, by use of a set of 90° spherical-sector bending plates. This arrangement minimized any background arising from the collection of the primary $K^-$ beam. The dispersed $K^+$ ions then entered a negatively biased detection box, where the ions impinged on a metal plate and produced secondary electrons. These secondary electrons were, in turn, accelerated toward a channel electron multiplier. The electron pulses from the detector were amplified and passed through a single channel analyser (SCA) in order to discriminate against electronic noise. The output of the SCA was converted into TTL pulses and counted with a multifunction I/O board in a PC-based data acquisition and control system. The magnitude of the ion-beam current, which was typically 1–6 nA in the interaction region, was monitored and used to normalize the yield of $K^+$ ions. Similarly, the photon intensity was monitored with a calibrated Si p–n junction photodiode and used for normalization purposes. The normalized $K^+$ signal is proportional to the photodetachment cross section and was used to investigate structure in the cross section.

Figure 3 shows the yield of $K^+$ ions produced when $K^-$ ions absorb photons in the energy range 21.0–24.5 eV. The photon energy scale has an estimated uncertainty of $\pm 10$ meV. A small correction was made to the scale to account for the Doppler shift associated with the moving ions. The dominant process is the non-resonant detachment of a single 3p inner-shell electron:

$$h\nu + K^-(3p^6 4s^2) \rightarrow K(3p^5 4s^2) + e^-. \tag{1}$$

The core-excited K atoms thus produced preferentially decay rapidly via the Auger process to form $K^+$ ions:

$$K(3p^5 4s^2) \rightarrow K^+(3p^6) + e^-. \tag{2}$$

The $K^+$ ion is detected and used to monitor changes in the cross section for process (1). The figure shows the non-resonant cross section rising over the whole energy range studied. The threshold energies for process (1) are equal to the energies of the $K(3p^5 4s^{2\,2}P_{1/2,3/2})$

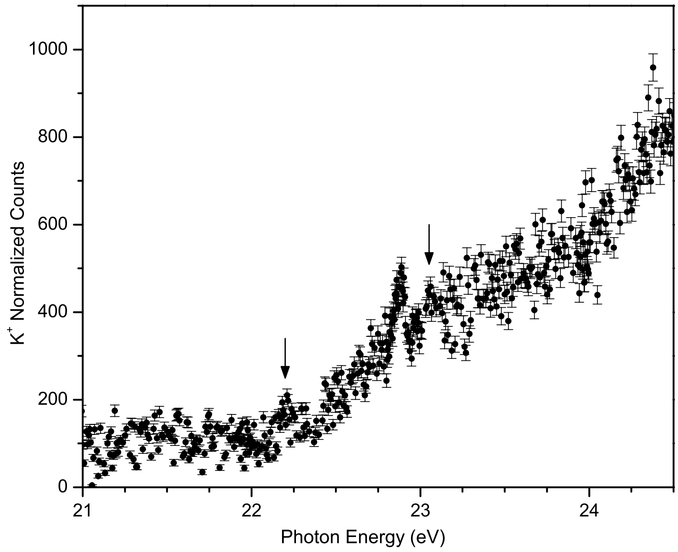


**Figure 3.** The yield of $K^+$ ions produced in photodetachment from $K^-$ in the photon energy range 21.0–24.5 eV

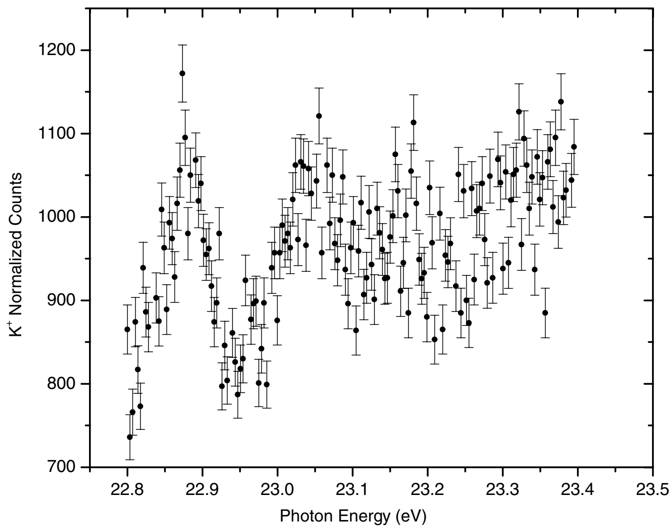


**Figure 4.** A higher resolution study of a portion of the cross section shown in figure 4. The dominant peak at 22.9 eV is a resonance associated with the $3p^5 4s5s6s\ ^1P^o$ core-vacancy state in $K^-$.

states relative to the energy of the $K^-(3p^6 4s^{2\,1}S_0)$ state. These energies are 19.22 eV ($^1S_0 \rightarrow {}^2P_{1/2}$) and 19.48 eV ($^1S_0 \rightarrow {}^2P_{3/2}$). It was not possible to observe these thresholds in the present experiment because, below about 20 eV, the photon flux was greatly reduced due to the large drop-off in efficiency of the grating used to monochromatize the synchrotron radiation.

Superimposed on the non-resonant cross section are resonances associated with double excitation of the $K^-$ ion. Figure 4 shows a portion of the cross section shown in figure 3 at higher resolution. It contains a single prominent resonance and many unresolved or partially resolved resonances. Typically, in the energy range of the present experiment, the resonances arise from states that are formed by the simultaneous excitation of a core and valence electron:

$$h\nu + \mathrm{K}^-(3\mathrm{p}^6 4\mathrm{s}^2) \rightarrow \mathrm{K}^{-*}(3\mathrm{p}^5 4\mathrm{s}n\ell n'\ell') \rightarrow \mathrm{K}^*(3\mathrm{p}^5 4\mathrm{s}n\ell) + \mathrm{e}^-. \tag{3}$$

Again, we detected the $K^+$ ions produced in the Auger decay of the intermediate core-vacancy excited state of the K atom that was formed in the autodetachment process. The prominent resonance at 22.880 eV appears to lie close in energy to the $3p^5 4s(^1P)5s$ core-vacancy state of K. It is proposed that the dominant configuration of this state is $3p^5 4s5s6s$, differing from the parent state by an extra 6s spectator electron. In this configuration, the outer electrons all reside in different shells and all are in non-penetrating s-orbitals. These conditions result in a poor overlap between the electrons involved in the process of autodetachment, leading to a rate that should be relatively small. The narrow width of this resonance is the result of its relatively long lifetime. In the region 20–22 eV there appear to be several unresolved resonances, which is to be expected since there are many core-vacancy states of K in this same region. Weaker resonances appear to be present at energies of approximately 22.2 and just above 23 eV (see the vertical arrows in figure 3).

We have estimated the resonance parameters of the prominent resonance by fitting it to a Lorentzian function. The resonance energy and width of the $K^-$ peak were determined to be 22.880(6) eV and 60(7) meV, respectively. The uncertainty in the width is from the fit to the Lorentzian function and the uncertainty in the energy is from the fit and our estimation of the contribution of the non-constant background to the total uncertainty. The error bars are reported at one standard deviation. In figure 5 we compare the energies and widths of the $3p^5 4s5s6s\ ^1P^o$ resonance in $K^-$ at 22.880 eV with the corresponding $2p^5\ 3s4s5s\ ^1P^o$ resonance in $Na^-$ [1] at 36.200(3) eV. The fitted width of the $Na^-$ peak is 34.7(2.1) meV. These widths correspond to lifetimes of 11(1) fs for the $K^-$ peak and 19(1) fs for the $Na^-$ peak.

In summary, we have used VUV synchrotron radiation to study the total cross section for photodetachment from the $K^-$ ion leading to the production of a $K^+$ ion over the photon energy range 21–24.5 eV. The yield of $K^+$ ions is proportional to the detachment cross section for production of K atoms with a single 3p core-vacancy since the latter states decay predominantly via Auger emission to produce $K^+$ ions. The focus of this work has been the investigation of resonance structure in the cross section due to the production and decay of core-vacancy excited states of $K^-$ involving the simultaneous excitation of a 3p core electron and a 4s valence electron.

The energies of resonances associated with core-vacancy states of $K^-$ with configurations that differ from corresponding core-vacancy states of K by the presence of a single spectator electron have been estimated for the purpose of identification. There appear to be resonances in the cross section close to the estimated energies. Unfortunately, there are so many relatively weak and broad close-lying resonances that it was impossible to distinguish them at the present level of energy resolution. A few resonances, however, were observed above the non-resonant background. The most prominent of these, the resonance at 22.880 eV, is identified with the decay of a $^1P^o$ core-vacancy state of $K^-$ with a configuration $3p^5 4s5s6s$. It is thought that the relatively narrow energy width of this state is due to the suppression of the autodetachment rate arising from the poor overlap of the active electrons that are both non-penetrating and in different shells. In a previous study of similar resonances in $Na^-$, we identified the corresponding core-vacancy state $2p^5 3s4s5s\ ^1P^o$. Again, the fact that the active electrons in both $K^-$ and $Na^-$ are in non-penetrating orbitals and different shells leads to relative stability of the core-exited states, and therefore a narrow line width.

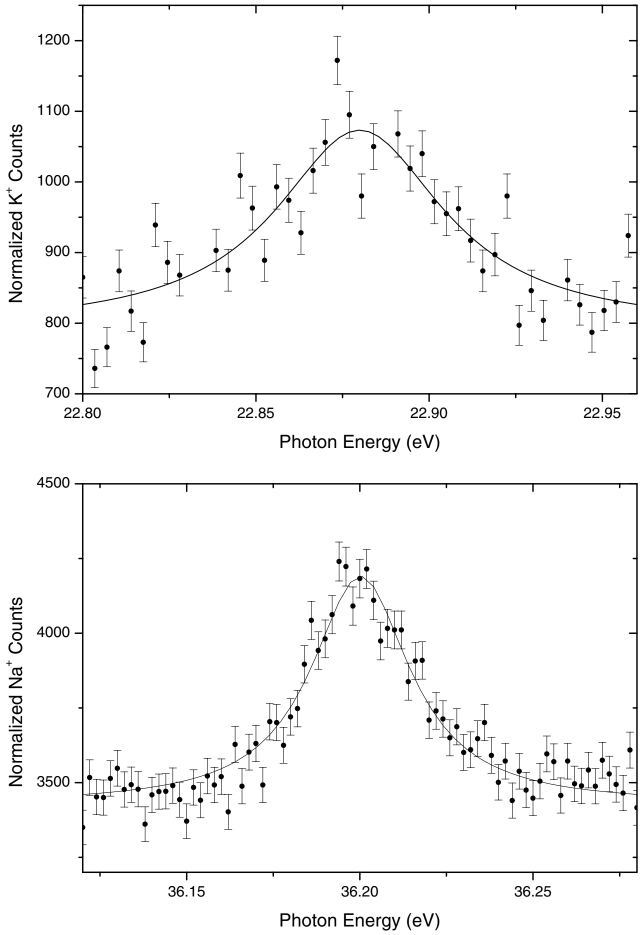


**Figure 5.** A comparison of analogous resonances in the K$^-$ and Na$^-$ ions. At the top is the peak arising from the decay of the 3p$^5$4s5s6s $^1$P$^o$ state in K$^-$ and at the bottom the peak is associated with the decay of the 2p$^5$3s4s5s $^1$P$^o$ state in Na$^-$.

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## References

[1] Covington A M *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** L735
[2] Kiyan I Yu, Berzinsh U, Sandström J, Hanstorp D and Pegg D J 2000 *Phys. Rev. Lett.* **84** 5979

[3] Petrunin V V, Volstad J D, Balling P, Kristensen P, Andersen T and Haugen H K 1995 *Phys. Rev. Lett.* **75** 1911
[4] Scheer M, Bilodeau R C and Haugen H K 1998 *Phys. Rev. Lett.* **80** 2562
[5] Andersen T 2004 *Phys. Rep.* **394** 157
[6] Pegg D J 2004 *Rep. Prog. Phys.* **67** 1
[7] Kjeldsen H, Andersen P, Folkman F, Christensen B and Andersen T 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** L353
[8] Berrah N *et al* 2001 *Phys. Rev. Lett.* **87** 253002
[9] Bilodeau R C, Bozek J D, Aguilar A, Ackerman G D, Turri G and Berrah N 2004 *Phys. Rev. Lett.* **93** 193001
[10] Aguilar A *et al* 2004 *Phys. Rev.* A **69** 022711
[11] Kjeldsen H 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** R325
[12] Andersson K T, Sandström J, Kiyan I Yu, Hanstorp D and Pegg D J 2000 *Phys. Rev.* A **62** 022503
[13] Pegg D J, Haselton H H, Thoe R S, Griffin P M, Brown M D and Sellin I A 1975 *Phys. Rev.* A **12** 1330
[14] Ralchenko Y, Jou F C, Kelleher D E, Kramida A E, Musgrove A, Reader J, Wiese W L and Olsen K 2006 NIST Atomic Spectra Database (version 3.1.0) URL http://physics.nist.gov/PhysRefData/ASD/index.html
[15] Covington A M *et al* 2002 *Phys. Rev.* A **66** 062710