

Laboratory measurements of Ca XIX dielectronic recombination satellites

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We report measurements of the astrophysically predominant $K\alpha$ emission from Ca XIX (He-like ion) and its satellite lines resonantly excited by dielectronic recombination (DR). We achieve an electron-energy resolution of 8 eV in a cryogenic electron beam ion trap, and determine the energies of the exciting electrons and the emitted photons up to the KLN ($n \leq 8$) manifold with 0.05 and 0.1% respective uncertainties. For the KLL satellites, energies agree very well with our predictions using the Flexible Atomic Code (FAC) and previous state-of-the-art calculations. Our calculations also agree with our experimental direct excitation cross sections for $K\alpha$ within their 10% uncertainty. We extract DR coefficient rates from our FAC calculations and find good agreement with values tabulated in the OPEN-ADAS database. Moreover, we compare FAC synthetic spectra, incorporating the DR atomic data benchmarked in the present work, with recent x-ray imaging and spectroscopy mission observations. This comparison highlights the contributions of DR satellites to the Ca XIX main lines.

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I. INTRODUCTION

The advent of high-resolution x-ray spectrometers on board space missions brought an urgent need for accurate laboratory data. While early x-ray space missions, like UHURU [1], Ariel V [2], and Heo-1 [3], provided only broadband spectra, later ones equipped with higher-resolution grating spectrometers such as Chandra [4,5] and XMM-Newton [6] enabled more detailed plasma diagnostics [7]. Such studies (see reviews [7,8]) included, e.g., electron temperature [9] and density distributions [10], bulk Doppler velocities of outflows [11], and estimates of turbulence velocities [11]. The analysis of such observations with spectral models crucially depends on the accuracy of the underlying atomic data. Recently, the soft-x-ray spectrometer microcalorimeter on board the ill-fated Hitomi satellite acquired high-resolution spectra of the Perseus cluster that allowed the characterization of the turbulent motion at its center [12] based on the broadening and Doppler shift of transitions of He-like ions. However, differences in theoretical atomic data used in the spectral codes ATOMDB/APEC [13], SPEX [14], and CHIANTI [15]

resulted in large discrepancies of up to 17% [16] for the iron abundance derived from the He-like z/w intensity ratio. Therefore, benchmark experiments are required to solve this problem. Nonetheless, the excellent resolution of Hitomi showed the overwhelming advantages of microcalorimeter-based x-ray astrophysics. A follow-up mission, the x-ray imaging and spectroscopy mission (XRISM) equipped with the Resolve microcalorimeter, is now operational, and has already delivered groundbreaking results, e.g., on the velocity distribution and thermal properties of the supernova remnants (SNR) N123D [17] and W49B [18], the bulk-gas motion in the Centaurus galaxy cluster [19], the accretion flow of the active galactic nucleus NGC 4151 [20], stellar winds in the binary system Cygnus X-3 [21], and the ionization state of the SNR Sagittarius A East [22]. Unfortunately, the gate valve in front of the XRISM detector malfunctioned in orbit, and observations have to take place through a beryllium window installed on it for prelaunch calibration. It strongly absorbs soft x-rays below 2 keV, hindering crucial diagnostics of, e.g., the Fe L -shell complex [19]. Thus, spectral diagnostics work only at higher energies, and rely on H-like and He-like $K\alpha$ lines of S, Ca, and Fe and their satellites [17]. One example is the Fe He-like $K\alpha$ transition used to analyze the bulk motion of the plasma at the Centaurus galaxy cluster [19]. The present experimental study benchmarks the $K\alpha$ satellites of He-like Ca XIX, which contribute to the collisionally excited $K\alpha$ lines of He-like Ca seen by XRISM.

Closed-shell He-like ions display very strong $n = 2 \rightarrow n = 1$ transitions, labeled following the Gabriel notation [23]. The most studied ones are the resonance line w ($1s2p^1P_1 \rightarrow 1s^2^1S_0$), the intercombination line composed of two transitions x ($1s2p^3P_2 \rightarrow 1s^2^1S_0$) and y ($1s2p^3P_1 \rightarrow 1s^2^1S_0$),

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as well as the forbidden line z ($1s2s^3S_1 \rightarrow 1s^2\ ^1S_0$). They are often accompanied by less intense Li-like satellite lines excited through dielectronic recombination (DR). Since the pioneering work of Massey and Bates [24] and Burgess [25] that showed the importance of DR for plasma emissivity, this atomic process was intensively studied both theoretically [26–29] and experimentally [30–52]. A compilation of $1s2\ell 2\ell'$ satellite lines is given by Ref. [53]. However, laboratory data on Ca XIX are scarce, stemming from Tokamak and accelerator experiments [54–56], and there is no comprehensive study about DR KLn energies and cross sections.

In this work, we report measurements of the DR KLn satellite emissions and the related collisional and resonant excitation of He-like Ca XIX taken with an electron-beam ion trap (EBIT). The high resolution of the electron-beam energy of FLASH-EBIT allowed us to accurately determine DR KLn electron and photon DR energies up to the $n = 8$ manifold through a two-dimensional (2D) fit. Relative collisional cross sections for DR and nonresonant excitation were also measured. These results are in very good agreement with state-of-the-art calculations obtained with the Flexible Atomic Code (FAC). Our FAC calculations were also compared with the values tabulated in the OPEN-ADAS [57] database. Moreover, we analyze the contributions of DR satellites to the Ca $K\alpha$ emissions using FAC collisional-radiative model predictions and compare them with recent XRISM spectra [18,19].

II. EXPERIMENT

A. Setup

FLASH-EBIT [58,59] was used to produce and probe He-like ions of Ca at the Max-Planck-Institut für Kernphysik in Heidelberg. A solid sample of the compound $\text{Ca}(\text{TMHD})_2$ [calcium bis(2,2,6,6-tetramethyl-3,5-heptanedionate)] was heated up to 90°C in the differentially pumped injection system of the device. The evaporated molecular beam enters the central trap region of the EBIT through narrow apertures, where the injected molecules are dissociated by an electron beam compressed by a 6-T magnetic field to a radius of tens of microns. The beam efficiently ionizes the resulting Ca atoms, and traps radially the generated ions.

To probe the various atomic processes of excitation and recombination leading to photon emission, we modulate the EBIT electron-beam energy using a duty cycle similar to our previous study done for He-like O [60]. It consists of a sawtooth cycle with a linear ramp-down and a symmetrical ramp-up between 2500 and 4700 eV. Since the Li-like and He-like ionization thresholds are ≈ 1160 and ≈ 5128 eV, the trapped ions are predominantly He-like ($\approx 80\%$), with a smaller Li-like fraction ($\approx 20\%$).

Photon emission following the electron-ion interactions was recorded using a silicon-drift detector (SDD), with a photon-energy resolution of around 140 eV of full width at half maximum (FWHM) at 3800 eV, and mounted at 90° relative to the electron-beam axis. Emission counts were recorded as a function of both electron-beam and photon energies, yielding two-dimensional spectral plots (for more details, see Ref. [60]).

In order to extract DR cross sections of He-like Ca, a sufficiently fast ramping scan of the electron energy in tens of milliseconds is necessary to avoid reduction of the parent ion population at the DR resonances (see Ref. [61]) due to the high recombination rate induced by the DR itself. On the other hand, we observed a larger electron-energy spread (≈ 15 eV) when ramping the beam energy this quickly, relative to scans over a few minutes (≈ 8 eV). This effect may be attributed to a variation in electron-beam density at fast and slow ramp cycles. Therefore, scans were performed with two ramp speeds, with periods of 500 s and 30 ms, each targeting a specific goal. We extract the DR resonant energies from the slow scan (500 s) (see Sec. IV A), while the DR cross sections were extracted from the fast scan (see Sec. IV B). In the slow-scan case shown in Fig. 1, we observe the entire DR KLn series of He-like Ca converging toward the $K\alpha$ emission. This emission mainly arises from direct excitation (DE), with a small contribution of resonant excitation (RE).

B. Background contribution

Alongside the He-like DR KLn series observed in Fig. 1, a DR KLL peak of Li-like Ca is clearly separable from the main He-like DR- KLL complex. We use this peak to infer the Li-like fraction, which is about 20%.

A contamination by Ar ions of nearly three times the concentration as the Ca ions was observed from the corresponding $K\alpha$ emission. This is likely caused by an air (1% Ar concentration) leak in the injection system, since the Ar lines were only visible when the injection was in operation. This is also in part due to the low vapor pressure of the solid Ca compound that we used in the present experiment. Nonetheless, the Ar and Ca $K\alpha$ emissions are 600 eV apart, and their interference is mostly negligible. The background between Ar and Ca $K\alpha$ consists of Ar $K\beta$ (≈ 3.7 keV) and M -shell transitions of Ni-like and nearby charge states of W (≈ 3.5 – 3.6 keV) [62], with Ar partly blending with Ca $K\alpha$ (see Sec. IV B). Moreover, a radiative recombination (RR) band closely coinciding with that of He-like Ar into the L shell is clearly visible, crossing through the Ca $K\alpha$ region between its KLL and the KLM features. However, as discussed in more detail in Appendix A, this feature is predominantly due to N -shell RR emission into ions of Ba, with only a small contribution of RR into He-like Ar. Emission from contamination of W and Ba arises because these elements are present in the electron-gun cathode (W-Ba matrix), and small amounts of its material are emitted by thermal evaporation and inevitably trapped with the Ca ions. However, these lines remain spectrally distinct from the Ca DR resonances and do not overlap with them (see Appendix A).

We also considered charge-exchange (CX) processes. Since the CX from He-like Ca produces Li-like ions, it cannot generate $1s-2p$ transitions given the $1s^2$ ground state. CX would only be relevant if H-like ions ($1s$) were present, which was not the case as the electron-beam energy was below the threshold for H-like ion production. Finally, although residual argon was present, the trap pressure remained below 5×10^{-10} mbar. Given that CX signatures are expected at significantly higher pressures [63,64], any contribution is negligible.

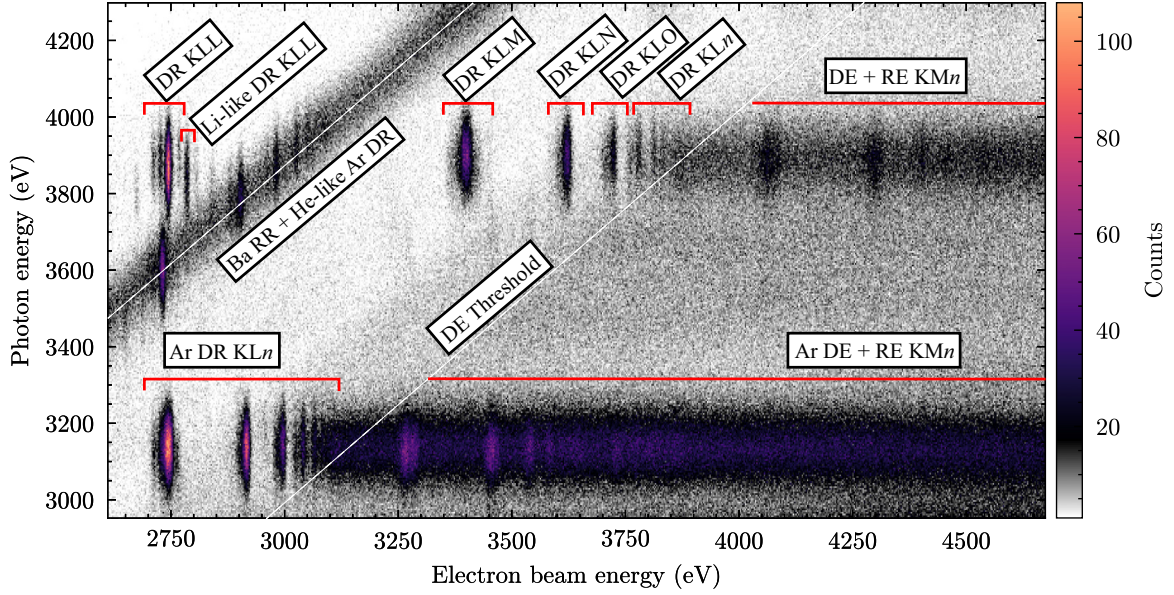


FIG. 1. Photon yield as a function of electron-beam energy and photon energy for a slow scan across the DR KLn structure of He-like Ca, as well as its DE and RE. A diagonal band of emission results from DR in He-like Ar, as well as L -shell RR into He-like Ar and N -shell RR into Ni-like Ba ions.

C. Energies and cross-section calibration

The SDD spectrum was calibrated by fitting well-known soft-x-ray lines of He-like Ca, Ar, and Ne for a wide range of energies, giving a calibration uncertainty of around 1.2 eV (0.03%) for a 1σ confidence band. More details on the calibration procedure can be found in Appendix B. The electron-beam energy calibration was made by matching three well-enough isolated DR peaks of He-like Ca, from KLL - j , KLN , and KLR , with their respective FAC values. The final calibration, combining the uncertainty components, resulted in an average energy uncertainty on the order of 1.6 eV (0.05%) for the 1σ confidence band. The fits to the KLL - j , KLN , and KLR peaks, together with the calibration curve, can be found in Appendix B. No significant contamination from other elements and Li-like Ca are expected at the DR KLn series that may shift the centroids. Therefore, the energy calibration is expected to be the main systematic uncertainty in both electron and photon energies.

To obtain experimental cross sections, a region of interest in the two-dimensional plot containing the Ca $K\alpha$ was projected onto the electron-beam energy axis. The projected intensity was normalized to the DR KLL of our FAC calculation including the experimental energy spread and correction factors for anisotropic photon emission (see Sec. III). We take into account the transmission of the 1- μ m-thick carbon filter in front of the SDD, as in earlier work [60,64]. Due to the relation between emissivity and cross sections [60], the summed counts were divided by $\sqrt{E_e}$, where E_e is the electron-beam energy. We estimate the systematic uncertainty of the cross-section calibration as follows: First, the uncertainty of the theoretical calibration was obtained by considering the convergence of the calculation in FAC (see Sec. III) when extending the configuration space. Contributions to the uncertainty from the fit to the KLL peak were considered in a similar manner as in Ref. [60], resulting in

a calibration uncertainty on the order of 5%. Different DR structures across multiple regions were also matched to the FAC calculations, and the standard deviation of the different calibration factors contributed to a systematic uncertainty of around 4%. Another 2% was considered to take into account the error in the anisotropy correction due to the depolarization effect of the cyclotron motion of the free electrons. The statistical uncertainty of the observations contributed to the majority of the total uncertainty, accounting for a contribution of an average value of around $\approx 8\%$. Combining all contributions, an average final uncertainty of $\approx 10\%$ was obtained for the measured cross sections presented in Sec IV B.

III. THEORY

FAC [65] was used to predict electronic levels and transition rates (radiative and autoionizing) of the ions of interest. The energy levels, autoionization A^a , as well as radiative rates A^r are calculated in FAC within the configuration-interaction (CI) approach. We evaluated resonant processes (DR and RE) according to the isolated-resonance approximation, i.e., without quantum interference effects between the nonresonant RR and resonances that connect the same initial and final states. Both DR and RE processes are described as a two-step process of an inverse autoionization process, also known as dielectronic capture (DC), followed by photon emission (DR case) or an autoionizing decay (RE case). In this case, the resonance strength (integral of the cross section) of each resonance is given by

$$S_{idf}^x = \int_0^\infty \sigma_{idf}^x(E_e) dE_e = \frac{\pi^2 \hbar^3}{m_e E_{id}} \frac{g_d}{2g_i} \frac{A_{di}^a A_{df}^y}{\sum_{i'} A_{di'}^a + \sum_{f'} A_{df'}^r}, \quad (1)$$

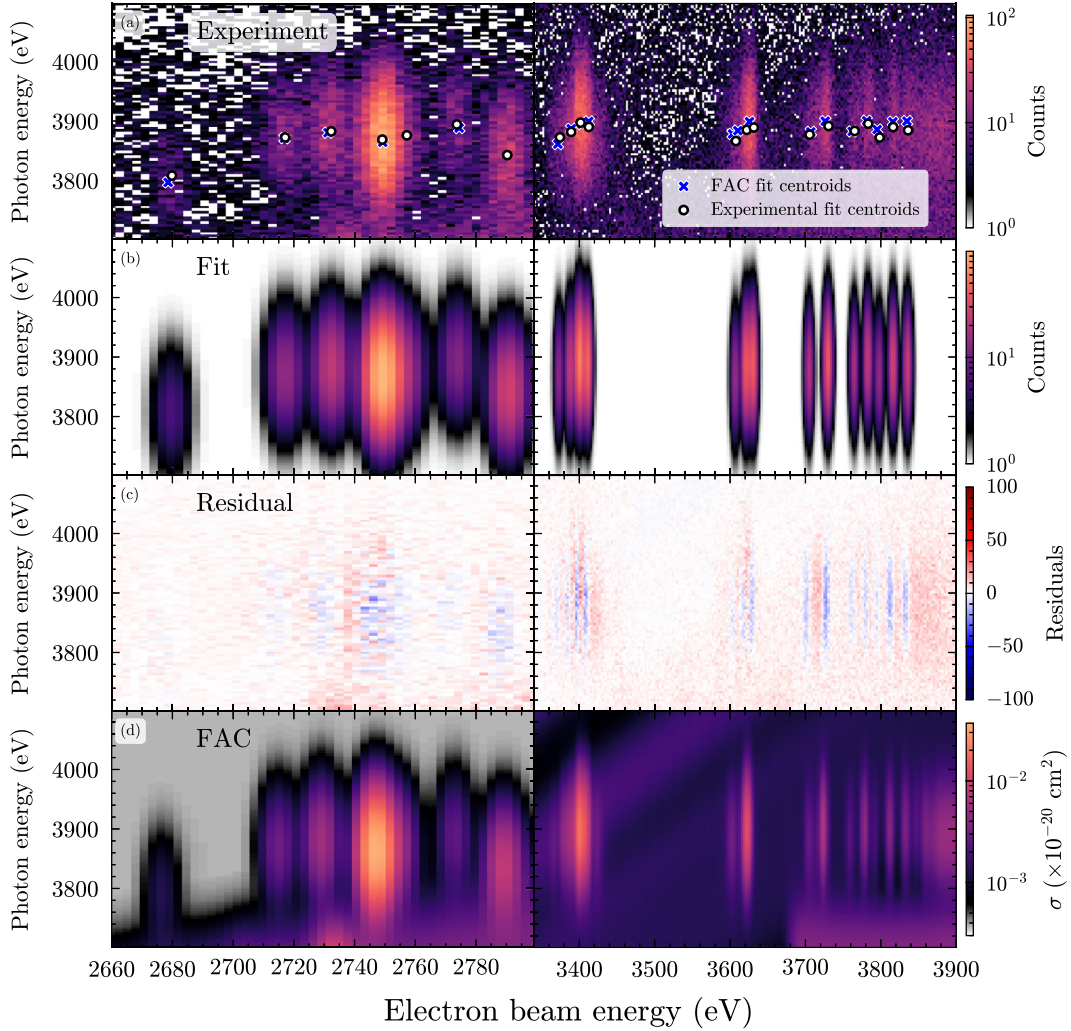


FIG. 2. Fit procedure for the DR emission plots. (a) Experimental results. Blue crosses mark the fit centroids of the FAC data; black circles mark those of the experimental data. (b) Plot of the experimental fit. (c) Residuals given by the fit procedure. (d) Plot of DR KLn FAC calculations convoluted with the experimental widths. The DR structures of He-like Ar as well as the RR and DE features of Ca, Ar, and Ba were also included for comparison with the experiment.

where $\sigma_{idf}^x(E_e)$ is the cross section of DR ($x = \text{DR}$, $y = r$), or RE ($x = \text{RE}$, $y = a$) as a function of the free-electron kinetic energy E_e for the process of inverse autoionization of the state i towards an intermediate state d followed by a photon decay (DR) or an autoionization decay (RE) to the final state f . E_{id} is the resonant energy of the electron-ion recombination between initial i and intermediate d states, with respective statistical weights g_i and g_d . m_e is the electron mass.

For the DR calculations we include the configurations of the ground state as well as singly and doubly excited states $1snl$ and $2lnl'$ up to $n \leq 15$. The DE and RR cross sections are obtained using the distorted-wave approximation from FAC including singly excited configurations up to $n_{\text{max}} = 10$. We also calculate higher n excitations to include their cascade contributions to the $K\alpha$ emission.

In order to identify features not belonging to the He-like ion, we calculate the Li-like structure with a set of configurations from the ground state $1s^22s$, singly excited- and doubly excited-state configurations $1s^2nl$ and $1s2lnl'$. Since the

Li-like DR emissions are weak, $n_{\text{max}} = 5$ was used. A complete map of the expected theoretical cross sections from DR, DE, and RR is shown in Fig. 2(c).

Due to the unidirectionality of the electron beam, photon emission is polarized and anisotropic [37,47,48,66]. For a direct comparison with the experimental data, we correct the theoretical cross section for the angular distribution, the anisotropic coefficient being calculated with the polarization module *FAC-pol*. Here, this coefficient is calculated based on the population distribution of the excited magnetic sublevels after the different excitation and recombination channels. Additionally, as the electrons follow a cyclotron motion within the beam due to the magnetic field, there is a depolarization effect dependent on the transverse electron energy [66–68]. In previous works, this value was observed for the same experimental conditions as this experiment, also validated with Herrmann's optical theory of electron beams [69], yielding a value between 400 and 500 eV [68]. In these conditions, the total anisotropy correction, for the observed energy range, can change from its nominal value by up to 2%. This value

was added to the cross-section uncertainties as a systematic uncertainty.

IV. RESULT ANALYSIS AND DISCUSSION

A. Experimental energy positions

Figure 2(a) displays a measurement of the Ca KLn DR resonances obtained with a slow scan of the electron-beam energy. Here, the two-dimensional spectrum was fitted with a linear combination of two-dimensional Gaussian functions using the MINUIT2 library of the ROOT analysis package [71] with a maximum likelihood algorithm. The FWHMs of the 2D-Gaussian functions were constrained to the FWHMs of 8 ± 1 and 140 ± 30 eV (shared across every fitted resonance) for electron and photon energies, respectively. These values were obtained previously for the isolated KLL - r resonance (see Appendix B). This is to ensure numerical stability during the fitting process. We assume no further broadening mechanism besides the instrumental resolution of the SDD and the electron-beam energy spread as Gaussian distributions [41,72].

Determining how many 2D-Gaussian functions are to be fitted is difficult, since tens of resonances can be unresolved in the data. For this work, we employed the K -means clustering method [73] to group the theoretical resonances into clusters weighted by their predicted resonance strength. The number of clusters n_c can be defined by how many features can be included without the minimum separation between clusters being less than the experimental width. The cluster centroids are then used as the initial parameters of the fit of n_c 2D Gaussians to the theory values (convoluted with the experimental widths of the photon and electron energy). The results of this fit are later used as initial parameters for the experimental fit. This ensures consistency between the fits to the theoretical and experimental results.

Applying this procedure to the KLn DR features allowed us to identify and fit resonances up to KLR ($n = 8$). A comparison of the experimental and fit results is plotted in Fig. 2. Figure 2(a) shows the experimental data, superimposed with the centroids obtained with the fit procedure (black circles). Fitted theoretical values convoluted by the experimental resolutions are compared, with the corresponding centroids also displayed as blue crosses. In general, the independently calibrated experimental data and the theoretical centroids mostly agree within the quoted uncertainties. As expected, there is better agreement at lower electron energies than at higher ones, since a growing number of unresolved resonances with n challenge the clustering method for peak fitting as well as the accuracy of the predictions.

The diagonal emission feature between 2800 and 3200 eV is due to RR of Ba and He-like Ar (see Appendix A), and displayed DR resonances of He-like Ar that were not fitted; KLL resonances of Li-like Ca resonance below 2800 eV were also excluded. Figures 2(b) and 2(c) show the functions obtained from the fitting procedure for the experimental and the convoluted FAC data. The calculations show more discernible structures at the higher energies of Fig. 2(c) than in Fig. 2(b). The observed intensities relative to the strongest KLL peak seem to be generally more intense than predicted. This could

result from the clear changes of the charge-state distribution taking place over the slow-scan range, with the He-like population increasing with the electron-beam energy. The centroids obtained from the experimental and theoretical data fits are compiled in Tables I and II for KLL and KLn ($3 \leq n \leq 8$), respectively. Listed uncertainties represent the quadratic sum of the energy calibration uncertainty (Sec. II C) with the 2D-fit statistical uncertainty.

While the KLL satellites of Ca have been theoretically studied by a few groups, currently no experimental or theoretical studies are reported for KLn ($3 \leq n \leq 8$). Table I compares the observed KLL satellite lines with the notation of Gabriel [70] and current state-of-the-art calculations, ordered by the electron energy of the resonances. As most of the experimental peaks have two unresolved satellites, each experimental value is compared with both theoretical values. Five experimental lines were observed, with the corresponding excited configurations being $1s2s^2$ ($p + o$), $1s2s2p$ (r , $t + s$), and $1s2p^2$ ($j + k$, $m + n$). These values were compared with the transition energies given by Refs. [26,28], and our FAC calculations. Values in parentheses in Table I indicate the relative difference between the theoretical value and experimental values. Transition energies included in Ref. [26] were calculated with both the AUTOLSJ [74] package and MZ perturbation method [75]. The AUTOLSJ package uses a scaled Thomas-Fermi-Dirac potential to estimate the radial wave functions with the SUPERSTRUCTURE code [76], where scaling parameters are optimized to the resulting energies. AUTOLSJ needs the level mixing from the previous code to calculate the autoionization rates. The MZ perturbation method contains a semirelativistic Z expansion of atomic parameters in powers of nuclear charge Z to calculate the energy levels taking into account relativistic effects and electron correlation. The calculations from Ref. [28] with a fully relativistic CI method include the frequency-dependent Breit interaction, relativistic nuclear recoil, and quantum electrodynamics effects, such as self-energy, vacuum polarization, and other nuclear-recoil contributions.

All predicted lines agree fairly well with the experimental results, deviating by less than 0.15% from the predictions of Ref. [28]. Only the two-electron-one-photon transitions p and o deviate from the most recent predictions by 0.06 to 0.22%, respectively; these seem to be underestimated in all predictions. Excellent agreement was found for the r , $j + k$, and $m + n$ lines ($j + k$ being the strongest KLL resonance), agreeing with most calculations within uncertainty, and m deviating by around 0.08%. FAC results are closest to those of MZ and CI + QED, while AUTOLSJ results tend to overestimate all lines by a few electron volts with respect to the theoretical trend. The largest deviations in the other works are seen in the n and m lines, where FAC and CI + QED values are 0.9 eV apart.

B. Experimental DR cross sections

Although the slow scan provided better electron-beam energy resolution, we noticed changes in the charge-state distribution when comparing upward and downward scans. In contrast, these are nearly identical for the 30-ms scan, confirming that the charge-state distribution remains constant

TABLE I. Fitted experimental electron (E_e) and photon energies (E_γ) (in eV) of KLL satellite transitions of He-like Ca labeled according to Gabriel's notation [70]. Results are compared with our FAC calculations and predictions obtained with the MZ and AUTOLSJ codes presented in Ref. [26] and the CI+QED method by Ref. [28]. $E\gamma$ -FAC values show photon energies fitted to the FAC data convoluted with the experimental width; FAC values denote the calculated transition energies. Since most lines are blended, we compare blended values from experiment and theory, with the relative difference shown in parentheses.

Label	Transition	E_e -exp	E_e -FAC	$E\gamma$ -exp	$E\gamma$ -FAC	FAC	AUTOLSJ	MZ	CI+QED
p	$1s2s^2\ ^2S_{1/2} \rightarrow 1s^22p^2\ ^3P_{3/2}$	2677.3 ± 1.9	2675.30	3808.4 ± 6.9	3791.8	3796.9 (−0.11%)	3800.7 (−0.01%)	3797.3 (−0.10%)	3797.6 (−0.09%)
o	$1s2s^2\ ^2S_{1/2} \rightarrow 1s^22p^2\ ^1P_{1/2}$					3791.8 (−0.24%)	3794.7 (−0.17%)	3792.1 (−0.23%)	3792.5 (−0.22%)
r	$1s2s2p^2\ ^2P_{1/2} \rightarrow 1s^22s^2\ ^2S_{1/2}$	2714.5 ± 1.8	2713.74	3872.5 ± 2.8	3870.8	3870.8	3874.4	3871.2	3871.2
t	$1s2s2p^2\ ^2P_{1/2} \rightarrow 1s^22s^2\ ^2S_{1/2}$	2729.6 ± 1.7	2727.93	3882.7 ± 2.4	3880.5	3884.9	3888.0	3884.8	3884.9
s	$1s2s2p^2\ ^3P_{3/2} \rightarrow 1s^22s^2\ ^2S_{1/2}$					3885.9	3889.5 (0.04%)	3885.9	3885.9
j	$1s2p^2\ ^2D_{5/2} \rightarrow 1s^22p^2\ ^3P_{3/2}$	$2746.4^a \pm 1.7$	2745.98	3868.8 ± 1.6	3862.3	3862.3 (−0.15%)	3865.7 (−0.06%)	3862.2 (−0.15%)	3862.3 (−0.15%)
k	$1s2p^2\ ^2D_{3/2} \rightarrow 1s^22p^2\ ^1P_{1/2}$	2754.5 ± 1.7	2753.51	3876.0 ± 4.2	3866.9	3866.9 (−0.13%)	3870.4 (0.04%)	3866.8 (−0.13%)	3866.8 (−0.13%)
n	$1s2p^2\ ^2S_{1/2} \rightarrow 1s^22p^2\ ^1P_{1/2}$	2770.9 ± 1.7	2771.21	3894.3 ± 3.7	3888.3	3893.0	3897.0	3892.1	3892.1
m	$1s2p^2\ ^2S_{1/2} \rightarrow 1s^22p^2\ ^3P_{3/2}$					3887.9 (−0.05%)	3890.9	3887.0 (−0.08%)	3887.0 (−0.08%)

^aUsed for the electron-beam energy axis calibration.

over the scan range. Figure 3 shows the cross sections at 90° obtained after the cross-section calibration procedure, as described in Sec. II C, to the sum of upward and downward scans. As in the slow scan, RR and DR from Ar and Ba also contaminate the fast scan, as seen in Fig. 3 between 2800 and 3300 eV. A small contamination of Li-like Ca is also observable by its respective KLL resonance below 2800 eV, as well as a possible trace of Be-like Ca at 2850 eV. The Ca RR band, expected at the Ca KLL structure, is not observed due to its low cross section, which falls below the scale of Fig. 2(c). A similar situation occurs for the nearby element Ar, where the apparent Ar RR band is, in fact, dominated by N -shell RR into Ba ions (see Appendix A).

Overall, the predicted DR features agree very well with our experimental results. Agreement is also found for the

DE cross section and RE KMn structure upon inclusion of residual contamination of Ar He-like $K\beta$ and Ca Li-like $K\alpha$ (see right side of Fig. 3). We resolve DR KLn resonances up to $n = 6$; beyond that, they blend together, and their resonance energies converge into the DE thresholds of the main line.

The experimental resonance strengths observed at 90° of each of the DR features are presented in Table III. Only the KLL , KLM , KLN , and KLO resonances were sufficiently isolated for a meaningful comparison with FAC predictions and other works. General agreement between the measurement and the FAC predictions for the DR structures (aside from KLL structure, which was used for normalization) is also shown with the inclusion of Li-like contamination. Although it is not possible to provide pure experimental He-like DR resonant strengths, the present FAC calculations can be

TABLE II. Same as Table I but for the KLn ($3 \leq n \leq 8$) satellite transitions. Since all resolved peaks are a blend of several resonances, we identify them by the leading one.

	Leading transition	E_e -exp	E_e -FAC	$E\gamma$ -exp	$E\gamma$ -FAC
KLM	$1s2s3s\ ^2S_{1/2} \rightarrow 1s^23p^2\ ^3P_{3/2}$	3370.3 ± 1.4	3368.20	3872.7 ± 3.4	3861.4
	$1s2p3s\ ^2P_{1/2} \rightarrow 1s^23s^2\ ^2S_{1/2}$	3385.2 ± 1.4	3385.88	3881.8 ± 2.4	3887.1
	$1s2p3p^2\ ^2D_{5/2} \rightarrow 1s^23p^2\ ^3P_{3/2}$	3397.7 ± 1.4	3400.34	3897.4 ± 1.8	3895.0
	$1s2p3d\ ^2F_{7/2} \rightarrow 1s^23d^2\ ^2D_{5/2}$	3408.6 ± 1.4	3409.16	3890.1 ± 2.0	3899.4
KLN	$1s2s4p^2\ ^2P_{1/2} \rightarrow 1s^24s^2\ ^2S_{1/2}$	3603.5 ± 1.7	3602.69	3866.4 ± 3.5	3878.3
	$1s2p4p^2\ ^2D_{5/2} \rightarrow 1s^24p^2\ ^3P_{3/2}$	3617.9 ± 1.7	3618.79	3885.2 ± 2.4	3883.9
	$1s2p4d\ ^2F_{7/2} \rightarrow 1s^24d^2\ ^2D_{5/2}$	$3627.3^a \pm 1.8$	3623.35	3889.2 ± 2.1	3899.1
KLO	$1s2s5p^2\ ^2D_{3/2} \rightarrow 1s^25p^2\ ^3P_{3/2}$	3701.3 ± 1.9	3703.68	3877.2 ± 2.2	3881.7
	$1s2p5d\ ^2F_{7/2} \rightarrow 1s^25d^2\ ^2D_{5/2}$	3726.4 ± 1.9	3723.07	3891.6 ± 1.8	3899.8
KLP	$1s2p6p^4\ ^2D_{5/2} \rightarrow 1s^26p^2\ ^3P_{3/2}$	3760.9 ± 2.0	3758.83	3883.4 ± 2.3	3882.6
	$1s2p6d\ ^2F_{7/2} \rightarrow 1s^26d^2\ ^2D_{5/2}$	3778.9 ± 2.1	3777.89	3895.5 ± 2.1	3900.5
KLQ	$1s2p7p^2\ ^2D_{3/2} \rightarrow 1s^27p^2\ ^3P_{3/2}$	3794.1 ± 2.1	3792.10	3872.3 ± 2.5	3885.8
	$1s2p7d\ ^2F_{7/2} \rightarrow 1s^27d^2\ ^2D_{5/2}$	3812.0 ± 2.1	3812.71	3889.9 ± 1.9	3896.5
KLR	$1s2p8d\ ^2F_{7/2} \rightarrow 1s^28d^2\ ^2D_{5/2}$	$3831.8^a \pm 2.2$	3831.59	3884.5 ± 2.0	3892.8

^aUsed for the electron-beam energy axis calibration.

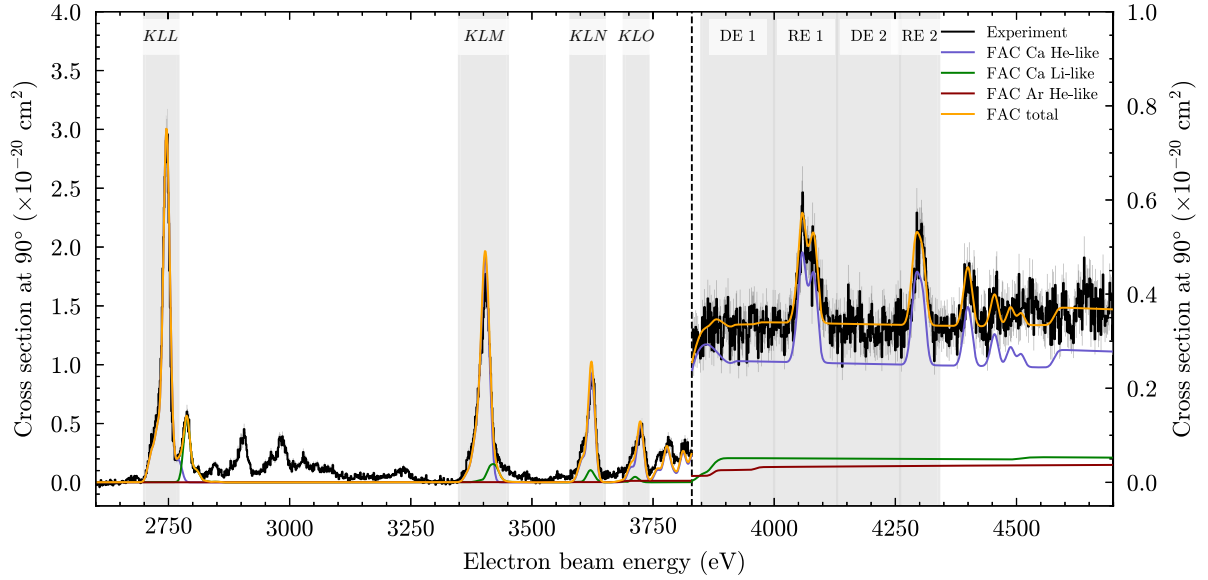


FIG. 3. Calibrated cross section (for photon emission at 90°) of He-like Ca DR KLn , DE, and RE as a function of the electron-beam energy from a fast scan. Orange and green lines represent FAC values for He-like and Li-like Ca. Gray regions mark the energy ranges used to calculate the DR and RE resonant strengths and DE integrated strengths.

compared with AUTOLSIJ and MZ calculations [26], which are represented in the table corrected for the anisotropy factor given by FAC. Overall, the AUTOLSIJ calculations align more closely with the FAC results, showing relative deviations of around 8%, whereas the MZ calculations exhibit deviations of approximately 23%.

C. DR rate coefficients

To directly compare our experimentally benchmarked FAC calculation with the rates retrieved from the OPEN-ADAS database, one of the most widely used in astrophysics, the theoretical data were converted into rate coefficients following Refs. [61,77]:

$$\alpha_{if}^{\text{DR}} = \frac{m_e}{\sqrt{\pi} \hbar^3} \left(\frac{4E_y}{k_B T_e} \right)^{3/2} a_0^3 \sum_d E_{id} S_{idf}^{\text{DR}} e^{-\frac{E_{id}}{k_B T_e}} \quad (2)$$

TABLE III. Experimental values of various Ca DR KLn resonance strengths and DE and RE integrated strengths measured at 90° in units of $10^{-20} \text{ cm}^2 \text{ eV}$. Energy ranges used for integration for both experiment and FAC calculations are indicated in Fig. 3. The resonance strength of the KLL resonances was used for normalization. Results are compared with our FAC calculations for He-like Ca with residual contribution of Li-like Ca and He-like Ar. Calculations from MZ and AUTOLSIJ codes for He-like Ca DR structure, presented in Ref. [26], and corrected for 90° , are also listed.

Structure	Energy region (eV)	Expt. ^a	FAC total	FAC Li-like	FAC Ar He-like	FAC He-like	AUTOLSIJ	MZ
<i>KLL</i>	2700–2770	63 ^b	62.986	0.107		62.879	67.962	73.487
<i>KLM</i>	3350–3450	52.4 ± 4.7	52.254	4.604		47.65	44.035	64.950
<i>KLN</i>	3580–3650	23.3 ± 2.4	21.291	2.155		19.136	20.890	25.298
<i>KLO</i>	3690–3740	13.1 ± 1.5	11.576	0.892	0.638	10.046	14.279	13.235
DE 1	3850–4000	48.8 ± 5.1	50.038	6.891	3.837	39.310		
DE 2	4130–4260	42.2 ± 4.4	43.316	6.451	4.417	32.448		
RE 1	4000–4130	51.2 ± 5.1	52.551	6.548	4.289	41.714		
RE 2	4260–4340	30.8 ± 3.1	32.127	3.882	2.745	25.500		

^aIncludes contributions from both He-like and Li-like charge states, with the exception of the *KLL* region.

^bUsed for cross-section calibration.

where E_y is the Rydberg constant in energy units, a_0 the Bohr radius, k_B the Boltzmann constant, and T_e the electron temperature.

Figure 4 compares the rate coefficients for He-like Ca from the OPEN-ADAS database with FAC values. Both *intermediate coupling* (IC) and LS coupling schemes are represented. FAC data were grouped and compared with IC and LS data according to the main type of transitions; i.e., the rates obtained from *KLL*, *KLM*, *KLN*, and *KLO* were compared with the database data relative to $1s2\ell2\ell' \rightarrow 1s^22\ell'$, $1s2\ell3\ell' \rightarrow 1s^23\ell'$, $1s2\ell4\ell' \rightarrow 1s^24\ell'$, and $1s2\ell5\ell' \rightarrow 1s^25\ell'$, respectively.

The rates from FAC are generally in good agreement with the OPEN-ADAS values in both LS and IC coupling schemes. Taking a representative temperature of $3.0 \times 10^7 \text{ K}$ (around the maximum of the rates), the IC and LS schemes predict higher than FAC by around 7 and 2%, respectively, while the IC scheme provides a value that is 5% higher than the

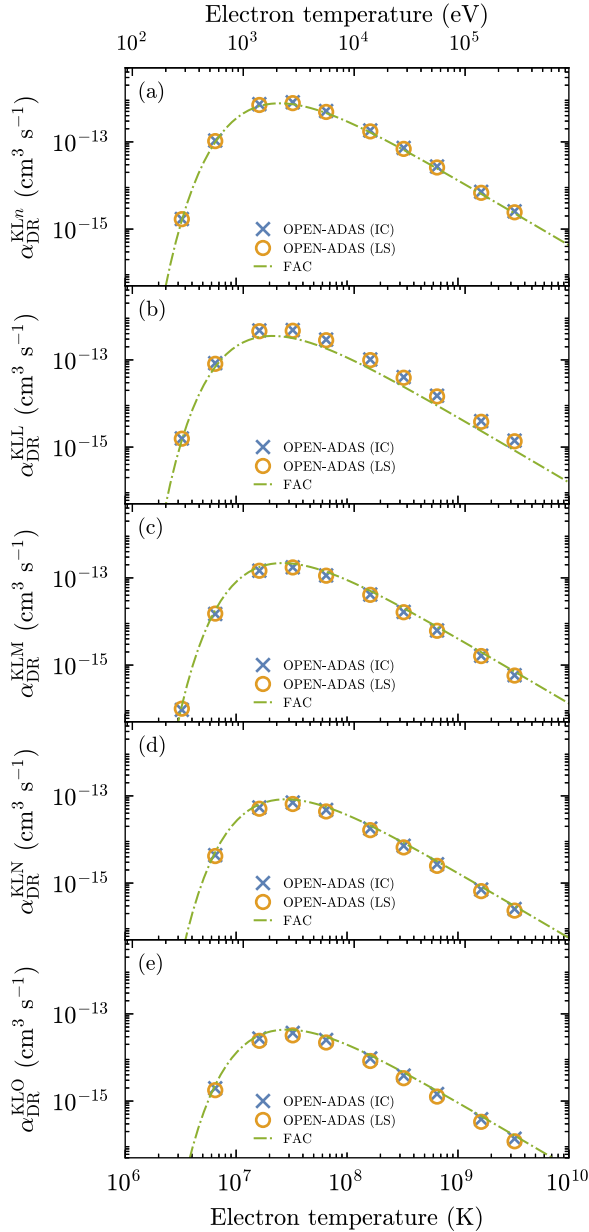


FIG. 4. K -shell DR rate coefficients of He-like Ca as a function of the electron temperature for (a) KLn , (b) KLL , (c) KLM , (d) KLN , and (e) KLO . FAC data are compared with OPEN-ADAS data in both IC and LS coupling schemes.

LS scheme. Regarding the different regions, both schemes tend to produce higher values than FAC by around 45%, while agreeing with each other by 4% in the KLL region. The opposite effect is observed in the rest of the structures, where both schemes produce lower values than FAC generally by around 20%, while deviating from each other by less than 15%. To make a quantitative comparison across the temperature axis, we present a small comparison for a lower and a higher temperature: 5.0×10^7 and 1.0×10^9 K. For the lower temperature, the total dielectronic recombination rate given FAC is higher than both IC and LS by 25%, with a divergence observed for the KLL structure and up to 50% for the remaining structures. The IC and LS schemes agree

mostly with each other within less than 10% across all structures. For the higher temperature, the total FAC rates are lower than the other schemes by less than 10%, with the IC and LS scheme deviating by around 5%. For the individual recombination structures, FAC yields lower values than the other schemes by 60%, while providing lower values for the other regions by around 20%, with the IC and LS scheme deviating from each other by around 7%. When comparing the integral of the entire presented temperature range for the total recombination rate coefficients, the IC and LS schemes provide 11 and 5% higher values than FAC, respectively, while the two schemes differ between each other by 5%.

D. XRISM observation

Several observations with XRISM show the $K\alpha$ complex of He-like Ca, as, e.g., in the Centaurus galaxy cluster [19], or the SNR W49B [18], where He-like Fe lines were used to infer their velocity distribution. Here we focus on the He-like Ca $K\alpha$ emissions around 3.9 keV. Figure 5 shows the (a) observations publicly provided by Ref. [19] for the Centaurus cluster and (b) observational data for the SNR W49B (East side) [18] downloaded from the NASA HEASARC repository [78].

In Fig. 5, we compare the two observations with the emission spectrum simulated with a steady-state collisional-radiative model (CRM) of the FAC-CRM package, which contains the present FAC atomic-data calculations. For simplicity, we consider a CRM consistent of a single-temperature model described by a Maxwellian electron-energy distribution. Calculations were done for electron temperatures in the ranges of 2.2–2.8 and 1.1–1.7 keV, as reported for the Centaurus galaxy cluster and the SNR W49B, respectively [18,19]. We input a typical electron density of 10^{-2} cm^{-3} for these objects [19] into our model. A three-ion model was adopted for Ca, including H-like, He-like, and Li-like charge states. Atomic structure included single and double excitations up to $n = 25$ and with the second excited electron up to $n = 3$ from the ground state, respectively, in the three ions. The populations of each level were determined by electron-collisional processes of DE, RR, CI, and DC and subsequent Auger and radiative cascades. CX processes were not included for simplicity. In the $K\alpha$ complex of He-like Ca, the only contamination expected arises from the He-like Ar $K\gamma$ line. This contribution was included, with the intensity inferred from the isolated $K\delta$ line (not shown). The DR emission comes from the radiative decay after the DC process, therefore by switching off this mechanism in the model the contribution of DR to the overall spectra can be directly investigated. Moreover, all simulations were broadened to observed FWHM of line w and normalized to its intensity. Figure 5(c) shows the DE and DR emissivities from FAC-CRM, and corresponding transition energies predicted by Refs. [79] and [28]. For the strongest DE and DR lines, particularly the j and k satellites, FAC calculations agree well with published theoretical data.

With $T_e \gtrsim 2.2$ keV as expected at the Centaurus cluster, the overall spectrum is dominated by the z , x , y , and w DE lines, with some residual contribution of DR satellites. At lower temperatures of 1.1–1.7 keV, as expected at SNR W49B, the DR satellite lines become stronger, in particular the j and k satellites near the z line. We note that the present CRM

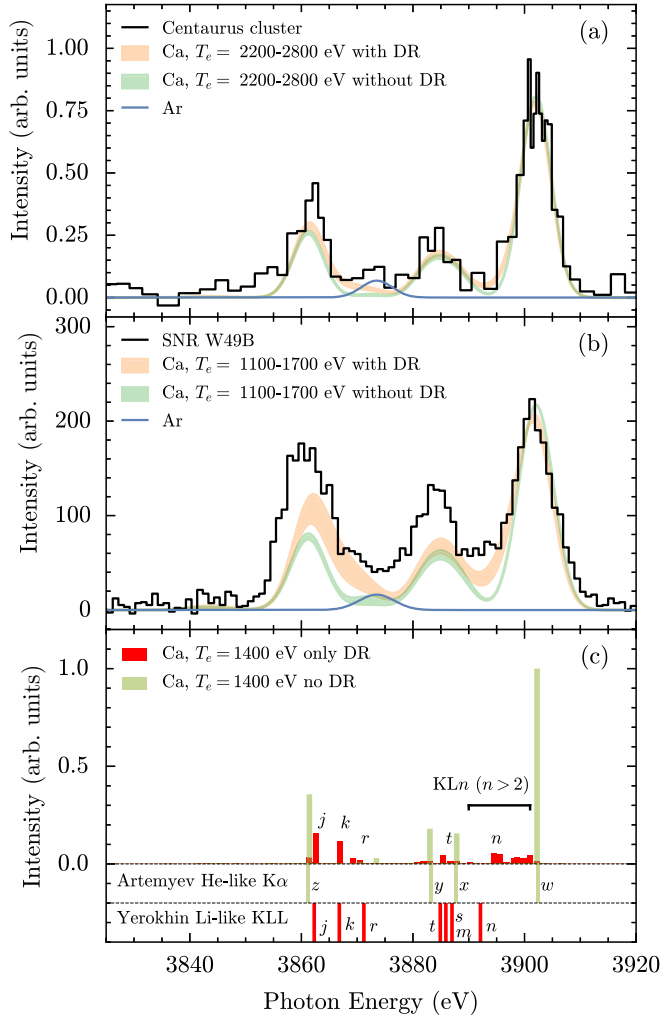


FIG. 5. XRISM observation of the (a) Centaurus galaxy cluster [19] and (b) SNR W49B [18] at Ca XIX $K\alpha$ (solid black lines). Comparison is made with FAC-CRM simulations (solid lines) for electron temperatures T_e (a) between 2.2 and 2.8 keV and (b) between 1.1 and 1.7 keV, showing full predictions (orange), as well as without DR contributions (green), and expected emission from He-like Ar (blue line). (c) Line emissivities at $T_e = 1400$ eV simulation. Below: He-like lines (green) and the Li-like KLL satellites (red) compared with energy calculations of Refs. [79] and [28], respectively.

modeling was performed specifically to illustrate these DR contributions to the Ca $K\alpha$ complex; a full modeling based on detailed astrophysical source parameters is beyond the scope of this paper. These results primarily serve to highlight the critical role of DR in modeling high-resolution XRISM observations.

V. SUMMARY AND CONCLUSIONS

The electron-ion collisional excitation of $K\alpha$ by dielectronic recombination, direct, and resonant excitation channels was studied in He-like Ca by measuring with EBIT x-ray spectra as a function of the electron energy. We resolved dielectronic resonances up to KLR ($n = 8$), and by fitting obtained their excitation energies and the photon energies emitted by these features. We compared them with FAC predic-

tions, and found, in general, good agreement outside blends at higher- n resonances. We also measured Li-like satellites of the KLL resonances and found that advanced predictions from the literature also reproduce them fairly well. In addition, we mitigated changes in the charge-state distribution using a fast energy scan to also determine DR, DE, and RE cross sections. The overall energy dependence, the shapes of the energy thresholds, and the relative strengths of the resonances also agree well with our FAC calculations. We determined experimental resonance strengths for KLL , KLM , KLN , and KLO , and compared them with the currently available theoretical literature. DR coefficient rates based on the FAC calculations were also compared with the data available in the OPEN-ADAS database for this astrophysical prominent ion, and a good agreement was found between the two.

By comparing synthetic spectra calculated from FAC, benchmarked against our measurements, with high-precision XRISM observations [19], we highlight the role of DR satellites blending with the Ca XIX $K\alpha$ lines. Close inspection of the region around z shows that the strong j and k DR satellites produce a noticeable change in the amplitude and symmetrical shape of the z line.

The present laboratory measurements provide valuable high-resolution benchmarks of the atomic databases included in spectral fitting models incorporated in ATOMDB [13], SPEX [14], and CHIANTI [15]. This is essential for analyzing spectra from present and future x-ray observatories such as the XRISM [19] and ATHENA [80] missions, and confirming the reliability of astrophysical plasma diagnostics derived from Ca lines.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: RADIATIVE RECOMBINATION VERIFICATION

As already mentioned in Sec. IV B and illustrated in Figs. 2(a) and 2(c), the Ca RR band into the L shell is too weak to be detected in the short exposure time spent at each energy during the scans, and the feature appearing at the location of the Ar RR band is actually dominated by N -shell RR of Ba ions. Barium, originating from the coating of the EBIT

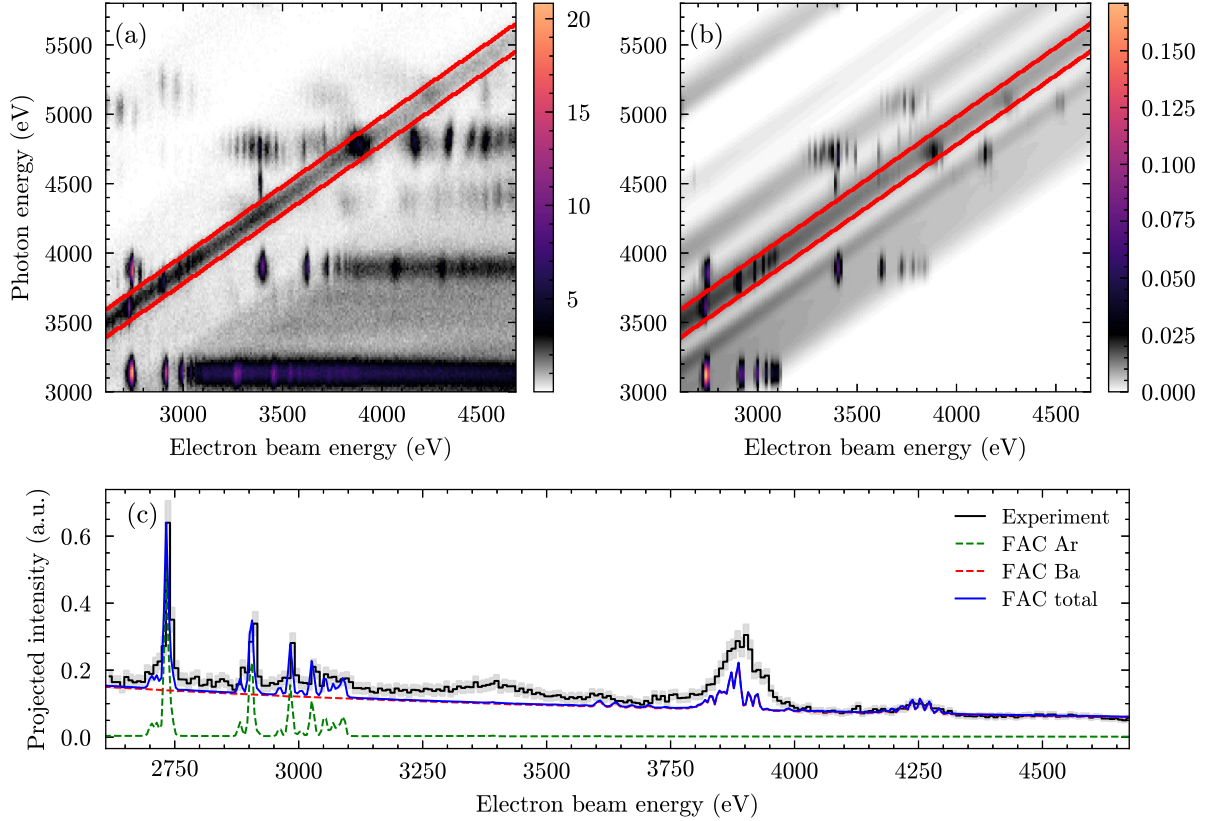


FIG. 6. (a) Photon yield as a function of electron-beam energy and photon energy, highlighting the RR band with a ROI. (b) Flexible atomic code cross sections for DR and RR of Ba, Ar, and Ca. (c) Corresponding ROI counts calibrated to cross sections.

cathode, is commonly present in EBIT observations. To minimize its influence, the trap is periodically dumped, purging all ions. This is effective because Ba ions fill up more slowly than the purposely injected Ca, and it takes approximately 13 s for the Ni-like Ba^{28+} (ionization energy of 970 eV) charge state to appear. This estimate is based on population-balance equations involving only RR and collisional ionization processes from a previous study [61]. We set the dump cycle to 33 s, as similar simulations with the same code indicate that this is required to produce 90% of He-like Ca. Therefore, the presence of $[\text{Ar}]3d^m$ ($m = 0, \dots, 10$) charge states of Ba is expected at the EBIT trap. Figure 6 shows an extended photon emission map of Fig. 1 together with FAC predictions [Fig. 6(b)], as well as the counts [Fig. 6(c)] for the RR ROI indicated there. Here, the experimental counts have been calibrated to match the area under the Ar KLM peak, based on FAC calculations of the same atomic process, including L -shell RR of He-like Ar and N -shell RR and LMn resonances of Ba ions. However, a comprehensive analysis of the complex $[\text{Ar}]3d^{10}$ DR LMn structure of Ba observed at higher energies is beyond the scope of this work. Nonetheless, these observations show how the blended-in RR band originates from these ions. Accordingly, our FAC calculations are limited to configurations with up to two unpaired electrons and holes in the $3d$ shell. The relative populations of the selected Ba ions used in our predictions are estimated based on population-balance simulations for the dump cycle. This approach effectively accounts for the missing charge states, as all relevant ions exhibit similar RR cross sections. Due to the much higher charged states

reached by the Ba ions under the present conditions, their RR cross sections are much larger than those of the Ar ions, and therefore Ba dominates the RR band region under the present experimental conditions.

APPENDIX B: PHOTON AND ELECTRON ENERGY CALIBRATION

To convert SDD channels into physical photon energies, a linear calibration was performed using a selection of soft-x-ray lines spanning a wide spectral range. Only well-known reference energies from He-like $K\alpha$ transitions from Ne, Ar, and Ca having clearly resolved profiles were included in the fit. We note that the offline calibration of the detector using neutral fluorescence lines was not possible, since the SDD is windowless and permanently attached under vacuum to the FLASH-EBIT. Thus, the calibration had to rely solely on the emission lines from highly charged ions trapped in the EBIT. Argon lines present due to a small leak were also used for the calibration. After the main observations, Ne was injected and excited under conditions similar to those of the main experiment. We also detect background lines from H-like and He-like O, Ne-like Fe, and several charge states of Ba and W (from the EBIT cathode), but do not use them for calibration. Line centroids from Gaussian fits with associated uncertainties were obtained. The fit of the three $K\alpha$ line complexes used for the calibration is displayed in Fig. 7. We use a shared width for all the Gaussians in each fit and subtract a constant background. In the case of Ar, the corresponding line is well

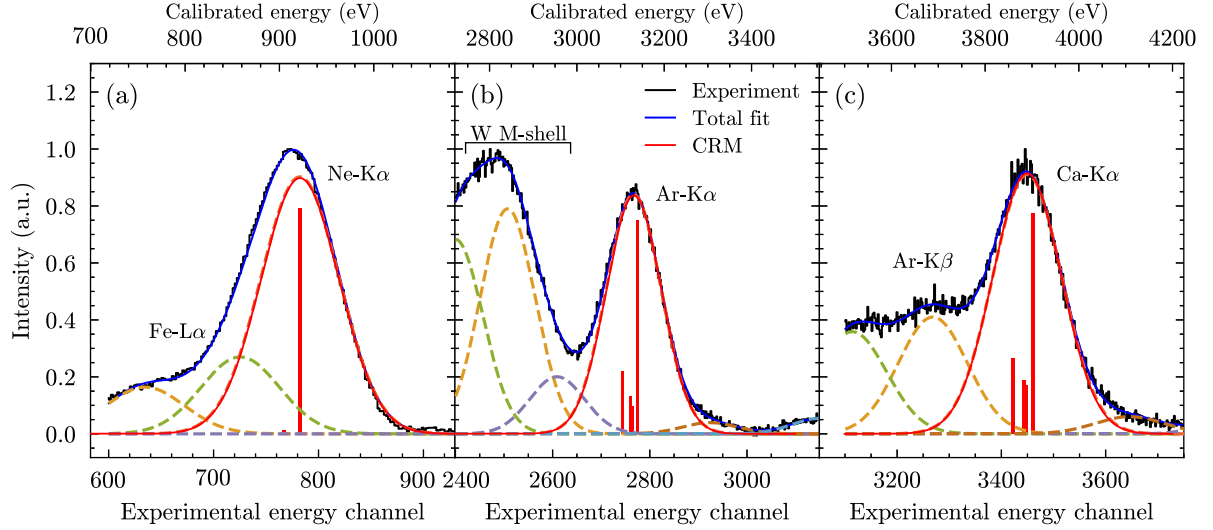


FIG. 7. Multiple Gaussian fits performed to the $K\alpha$ line complexes of (a) He-like Ne, (b) Ar, and (c) Ca. Experimental data (blue curve) and total fit (red dashed lines) are shown vs uncalibrated detector energy. Top axis: Calibrated photon energy. The relative emissivities of the $K\alpha$ lines are represented by the vertical red bars, as well as the corresponding Gaussian convoluted emission profile (solid red line).

TABLE IV. Experimental photon energies (channels), corresponding He-like energies (eV) compiled at the NIST database, and relative intensities used in the calibration. The values of $K\alpha$ presented in the table reflect the centroid value of fits to synthetic spectra generated for the calibration lines with their relative intensities. The NIST calibration lines are taken from accurate theoretical calculations from Ref. [81] for Ne, and from Ref. [79] for Ar and Ca. Their relative intensities were calculated with the FAC-CRM package for the EBIT conditions for each individual element. Measurements of each He-like line are also listed with the respective uncertainty given in parentheses.

Element	Transition	Experimental (arb. units)	Calibration lines (eV)	FAC (eV)	Line measurements (eV)	Ref.	Rel. intensity
Ne	w	782.30	922.09	921.99	922.124(34) 922.148(82)	[82] ^a [83] ^b	0.979
	x		n.l. ^c	914.38			<0.001
	y		914.68	914.19			0.005
	z		905.06	904.03			0.016
	$K\alpha$		921.78				
Ar	w	2771.22	3139.58	3139.49	3139.5927(76) 3139.5810(92) 3139.552(37) 3139.57(25)	[84] [85] [86] [87]	0.65
	x		3126.28	3125.54	3126.283(36) 3126.37(40) 3128(2)	[86] [87] [88]	0.08
	y		3123.53	3122.82	3123.521(36) 3123.57(24)	[86] [87]	0.11
	z		3104.15	3103.01	3104.1605(77)	[89]	0.19
	$K\alpha$		3130.26				
Ca	w	3449.55	3902.38	3902.25	3902.19(12) 3902.43(18)	[54] [90]	0.55
	x		3887.76	3886.98	3887.63(12)	[54]	0.13
	y		3883.32	3882.58	3883.24(12)	[54]	0.12
	z		3861.21	3860.04	3861.11(12)	[54]	0.19
	$K\alpha$		3890.20				

^aFrom 36 Chandra high-energy-transmission-grating observations. We assume no line contamination from other He-like lines. The CODATA 2018 [91] recommended value of $hc = 1.23984198 \times 10^{-6}$ eV/m was used for conversion.

^bSame as previous, but for the interstellar medium surrounding Cyg X-2.

^cNot listed in NIST ADS or Ref. [81].

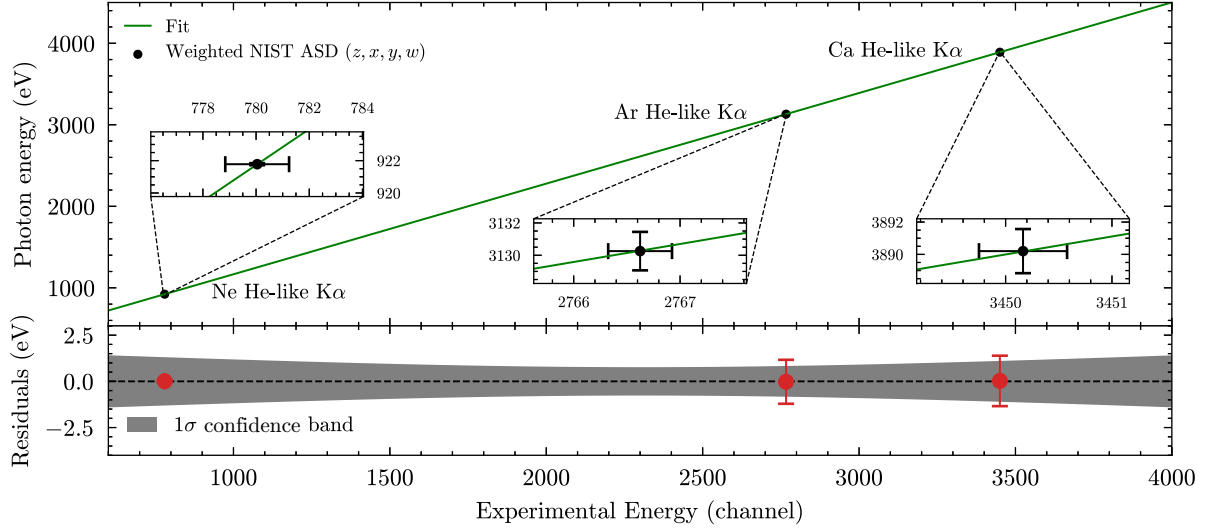


FIG. 8. Linear calibration fit using lines from Ne, Ar, and Ca. Error bars (see insets): Uncertainties in fitted line centroids (horizontal) and theoretical energies for calibration (vertical); residuals are shown at the bottom.

isolated, yielding a very low statistical error. Below the main Ar feature, background lines attributed to Co-like to Cu-like M -shell emission of W ($n_i = 4, 5, 6 \rightarrow n_f = 3$) [62] appear. For Ne, we notice some asymmetries in the low-energy tail of the main Gaussian. In this case, a shift of the centroid observed in the overall best fit seems to be due to a second Gaussian peak nearby. Such Gaussians arise from known contamination by H-like O and Ne-like Fe, leading to $K\beta$ and $L\alpha$ emission around ≈ 775 and ≈ 850 eV, respectively. A higher uncertainty for the centroid of the Ne $K\alpha$ feature was taken into account. On the left side of the main Ca $K\alpha$ lines are features attributed to the $K\beta$ lines of Ar, around ≈ 3680 eV.

Table IV lists measured detector positions (in channels) and corresponding reference energies used for calibration. Only transitions with reliable literature values compiled at the NIST ASD (except for the Ca lines) were used for calibration. The Ne lines at ADS NIST are theoretical values retrieved from Ref. [81], and for Ar and Ca from Ref. [79]. For the final calibration line of each element, an effective value for the $K\alpha$ line complex was calculated by fitting the emission spectrum obtained with a steady-state FAC-CRM for the experimental conditions, with the respective transition energies replaced by

those used for calibration and emissivities given by the FAC calculations. The weights obtained for each line are reported in Table IV. Energies for z , x , y , and w were also calculated with FAC, and agree within 1.4 eV with the theoretical ones used for the calibration, with the FAC values generally underestimating the values from Refs. [79,81]. For the cases of Ar and Ca, the FAC w values agree with the QED-based values of Ref. [79] within < 0.15 eV. Several laboratory observations of the $K\alpha$ lines for these elements were also compiled in the table for reference. Although high-precision laboratory observations are known for Ar and Ca, to the best of our knowledge, only wavelength measurements of Ne lines from astrophysical observations are currently available. Only the w line has been reported as the total $K\alpha$, which might be attributed both to the energy closeness of the lines and to the expectation that under those plasma conditions, other He-like lines are suppressed.

A least-squares regression weighted by uncertainties yielded the linear calibration function shown in Fig. 8. The abscissa uncertainties are taken from those of the fitted centroids, which presented a fit uncertainty of around 1.2 eV for Ne and less than 0.5 eV for Ar and Ca, while for the ordinate, the uncertainties from using FAC-CRM to weight the $K\alpha$ lines

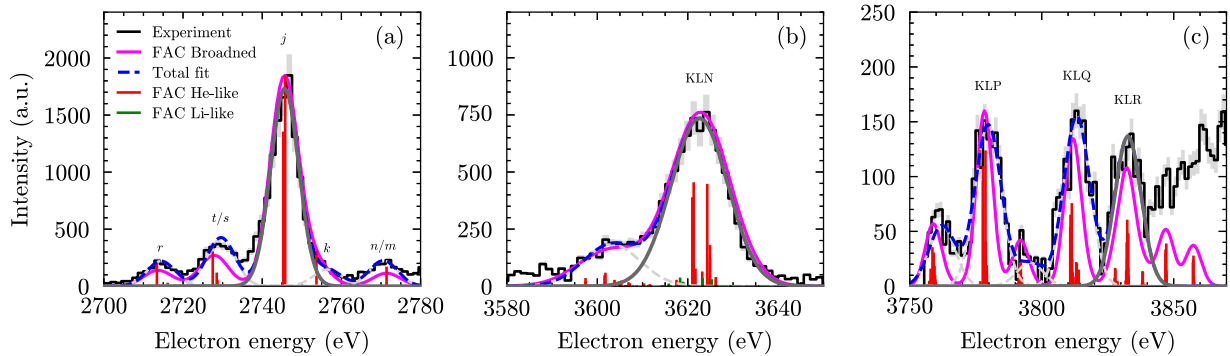


FIG. 9. Multiple Gaussian fits to the (a) KLL - j , (b) KLN , and (c) KLR peaks. Experimental data (black) are compared with convolved FAC spectra (pink) from both He-like (red sticks) and Li-like ions (residual green sticks in KLN). Total fit (blue) contains the Gaussian peak (bold gray) used for calibration in both experiment and convolved FAC spectra.

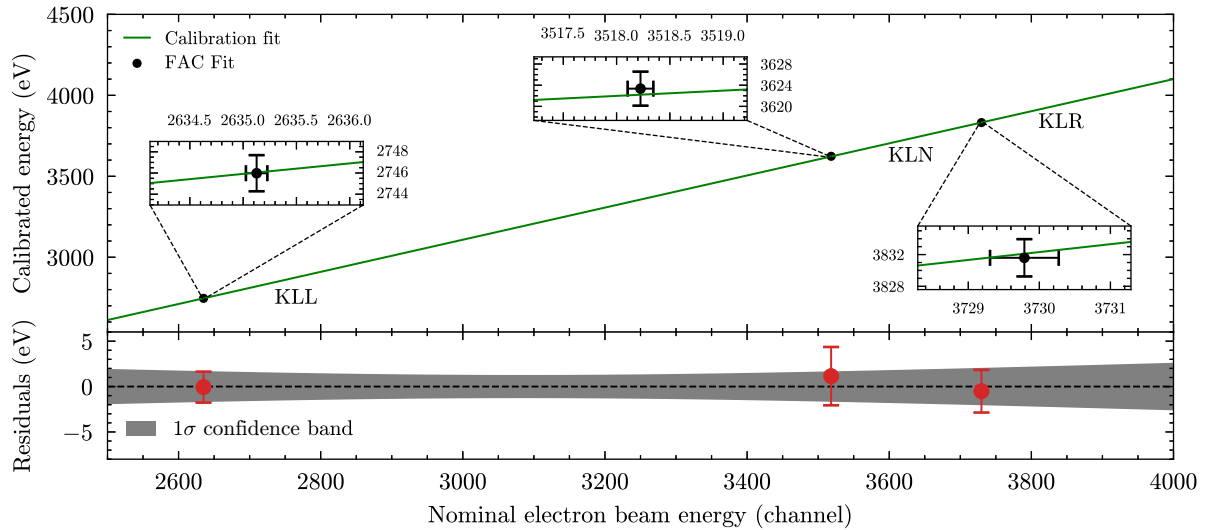


FIG. 10. Linear calibration fit using DR resonances from *KLL j*, *KLN*, and *KLR*. Error bars (see insets): Uncertainties in fitted line centroids (horizontal) and theoretical energies for calibration (vertical); residuals are shown at the bottom.

dominate. To estimate them, a conservative value of 20% was then used to vary the FAC-CRM line emissivities for each line. The highest changes of the effective centroid were taken as uncertainties for the transition energies of the calibration lines. In Ar and Ca the $K\alpha$ complex partially blends the x , y , and z lines, and the total uncertainty goes slightly over 1 eV. In Ne, the $K\alpha$ complex is dominated by w , and the centroid variations introduce an error of < 0.1 eV. The calibration line presented in Fig. 8 has residuals of 0.1 eV for Ar and Ca, and 0.01 eV for Ne. This makes us confident in the linear calibration of the SDD detector. We also noted that using the measured values of He-like lines listed in Table III for calibration instead of NIST values did not change either the linear calibration function or its uncertainty. The final uncertainty in the photon calibration includes the statistical uncertainty from the fit of the experimental reference lines, as well as the estimated uncertainty from the theoretical reference lines. The 1σ confidence interval for the calibration fit is represented as the uncertainty band in the residuals shown in Fig. 8. This, combined with the centroid uncertainty from the peak fitting, yields the total uncertainties in experimental photon energies shown in Tables I and II.

The nominal electron energy derived from several high-voltage power supplies was converted to an electron-energy

scale also using a three-point linear calibration. Owing to the absence of published DR resonant-energy values for He-like Ca, the calibration relies on FAC calculations as reference values. The calibration points were chosen to correspond to the peaks *KLL-j*, *KLN*, and *KLR* to represent a broad energy. The respective fits are shown in Fig. 9. As these peaks are still composed of multiple resonances, a Gaussian fit was made to a theoretical spectrum folded with the experimental resolution to match the fitted experimental centroids. The contamination from DR of Li-like Ca was taken into account in the theoretical spectrum, particularly for the centroid estimation of the *KLN* peak. The linear calibration resulting from the least-squares regression is presented in Fig. 10. The uncertainty associated with each experimental centroid uncertainty in Fig. 10 includes a horizontal error bar representing the statistical uncertainty from the fit (see Fig. 9), and a vertical error bar corresponding to the reference theoretical uncertainty of 0.05% combined with fit uncertainty to the convolved FAC spectrum, which is also approximately 0.05% on average. As in the photon-energy calibration case, the 1σ confidence band shown in the residual plot is considered as the electron-energy calibration uncertainty, with an average value of 1.6 eV (0.05%). The isolated resonance *KLL-r* shown in Fig. 9 was used to determine the electron-energy FWHM.

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