Comprehensive Laboratory Measurements Resolving the LMM Dielectronic Recombination Satellite Lines in Ne-like Fe XVII Ions

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ABSTRACT

We investigated experimentally and theoretically dielectronic recombination (DR) populating doubly excited configurations 3/3l (LMM) in Fe XVII, the strongest channel for soft X-ray line formation in this ubiquitous species. We used two different electron beam ion traps and two complementary measurement schemes for preparing the Fe XVII samples and evaluating their purity, obtaining negligible contamination effects. This allowed us to diagnose the electron density in both EBITs. We compared our experimental resonant energies and strengths with those of previous independent work at a storage ring as well as those of configuration interaction, multiconfiguration Dirac-Fock calculations, and many-body perturbation theory. This last approach showed outstanding predictive power in the comparison with the combined independent experimental results. From these we also inferred DR rate coefficients, unveiling discrepancies from those compiled in the OPEN-ADAS and AtomDB databases.

Keywords: atomic data — atomic processes — line: formation — methods: laboratory: atomic — plasmas — X-rays: general

1. INTRODUCTION

Iron, the heaviest among the abundant chemical elements, has strong L-shell transitions that dominate the X-ray spectra of astrophysical hot (megakelvin temperature regime) plasmas in the range of 15 – 18 Å. Due to its closed-shell configuration with a high ionization potential of 1260 eV, Fe XVII (Ne-like Fe+16) is a very stable and abundant species under these conditions. Collisional excitation of the 3d → 2p and 3s → 2p transitions in this ion generates the strongest observed lines in the X-ray spectra (for an overview, see Brown (2008) and references therein). These, together with less intense L-shell transitions from Fe in other charge states, e.g., Fe XVI (Na-like Fe+15), provide means for diagnosing the physical conditions of those plasmas (Paerels & Kahn 2003). Therefore, over many years numerous laboratory measurements have aimed at providing accurate values of the wavelengths and relative intensities of L-shell transitions in Fe XV-XIX (May et al. 2005), Fe XVI (Graf et al. 2009), Fe XVII (Laming et al. 2000; Beiersdorfer et al. 2002, 2004; Brown et al. 2006; Gillaspy et al. 2011; Shah et al. 2019), Fe XVIII-XXIV (Brown et al. 2005; Graf et al. 2000; Beiersdorfer et al. 2002, 2004; Brown et al. 2006; Chen et al. 2009), Fe XXI – Fe XXIV (Chen et al. 2005), Fe XXIV (Gu et al. 1999; Chen et al. 2002), and Fe XXI-XXIV (Gu et al. 2001). These works have revealed significant discrepancies with theory; well-known problems include the 3C/3D line ratio in Fe XVII (Bernitt et al. 2012; Kühn et al. 2020) and the Fe solar opacity issue (Nagayama et al. 2019). Moreover, it is expected that updated atomic data on Fe L-shells could resolve disparities among collision models used for predicting the Fe abundance (Mao et al. 2019) in low-temperature (and low-mass) elliptical galaxies (Yates et al. 2017; Mernier et al. 2019).
A recent review of astrophysical diagnostics of Fe L lines can be found in Gu et al. (2019, 2020).

Dielectronic recombination (DR) is the dominant photorecombination channel for Fe XVII in such plasmas. In the case of DR LMM, this means the capture of an electron into a vacancy of the M shell with a simultaneous, energetically resonant electron L–M excitation. The resulting doubly excited state can either autoionize, resulting in resonant excitation ((Shah et al. 2019) and (Tsuda et al. 2017) for Fe XVII and Fe XV-XVI), or radiatively decay, completing the recombination:

$$\text{Fe}^{16+} (1s^22s^22p^6) + e^{-} \rightarrow \text{Fe}^{15++} (1s^22l^23l''3l''') \rightarrow \text{Fe}^{15++} (1s^22s^22p^63l''') + h\nu \ (1)$$

Among the various processes exciting L–M emission, DR produces strong "satellite" transitions very close to the main lines due to the perturbation caused by the added spectator electron (Dubau & Volonte 1980; Clementson & Beiersdorfer 2013). Such lines were seen with the Chandra X-Ray Observatory in spectra from stellar coronae, like those of Capella and Procyon, and are used for plasma temperature determination (Beiersdorfer et al. 2018; Gu et al. 2020). DR also strongly influences plasma ionization equilibrium (Dupree 1968). It is thus crucial to accurately know these dielectronic satellites when diagnosing temperatures using collisional-radiative models (Savin & Laming 2002; Dudík et al. 2019), such as AtomDB (Foster et al. 2012) and SPEX (Kaastra et al. 1996), or with the help of atomic databases like CHIANTI (Dere et al. 2019) and OPEN-ADAS.  

Except for direct observation of DR 3l’l’’ and 3l’d’l’’ satellites in Fe XXII-XXIV (Gu et al. 2001), no laboratory wavelengths or intensities of Fe DR L-shell satellites are available, as mentioned in Beiersdorfer et al. (2014). Only recently have DR cross sections for the 3lnl’’ series for Fe XVII been published, with the purpose of investigating the 3d → 2p and 3s → 2p line ratios above the collision excitation threshold (Shah et al. 2019). These data benchmark the SPEX model and provide constraints on the global fit of Capella spectra (Gu et al. 2020). Continuing those works, we focus on the DR 3l’l’’ (LMM) satellites of Fe XVII, and provide experimental resonant strengths and rate coefficients. Similar measurements were previously done for Au (Schneider et al. 1992), Xe (DeWitt et al. 1992), and more recently for Si (Lindroth et al. 2020).

In this work, we remeasured previously studied Fe XVII LMM region by our group (see Shah et al. (2019)) with another electron beam ion trap (EBIT), PolarX-EBIT (described in Micke et al. (2018)). By using a modified measurement scheme, we obtained higher electron collision energy resolution compared to that in previous works. We also simulated the dynamical charge-state distribution for the present experimental conditions in order to exclude a possible large depletion of Fe XVII ions due to DR. Furthermore, we inferred the electron beam density for both devices, obtained experimental integrated resonant strengths from the two different measurement schemes, and compared them with those of earlier photorecombination studies performed at the Heidelberg Test Storage Ring (TSR) (Schmidt et al. 2009).

In addition, our new calculations based on multiconfiguration Dirac–Fock (MCDF) equations and our previous ones based on the Flexible Atomic Code (FAC) were compared with configuration interaction predictions by Nilsen (1989). Finally, our experimental and theoretical resonant strengths were converted to DR rate coefficients for a few electron temperatures and compared with those available in the OPEN-ADAS database, as well as with those in Zatsarinny et al. (2004), which are included in AtomDB (Foster et al. 2012), a spectral modeling code widely used in the X-ray astrophysics community.

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1 https://open.adas.ac.uk

2. EXPERIMENT
For accurate values of DR intensities, we relied on two complementary measurements made on two different EBITs. Previous work with FLASH-EBIT at Max-Planck-Institut für Kernphysik in Heidelberg is reported in detail in Shah et al. (2019). We summarize here the method and emphasize the differences with the new measurements performed with PolarX-EBIT. In both devices, Fe atoms were injected into the trap and ionized by a magnetically compressed monoenergetic electron beam with a radius of tens of micrometers. Its negative space-charge potential confined the ions, allowing stages of high ionization to be reached.

The DR LMM resonances appear at electron energies below the Na-like ionization threshold into Ne-like. This requires one to first produce (breed) the Fe XVII of interest before quickly changing the interaction energy to the values to be probed, as described below. Since DR depletes the Ne-like population into Na-like if the probe time is too long, we quantify this small effect in Sec. 4. Our recorded signal, X-ray emission including the contribution from DR, was observed at 90° relative to the beam axis with a silicon drift detector at both EBITs. Its photon energy resolution was around 120 eV FWHM at 6 keV.

2.1. FLASH-EBIT Measurements

The electron beam energy was at 1.15 keV for a 0.5 s breeding time, followed by a linear ramp-down from 1.15 to 0.3 keV within 40 ms and a symmetric ramp-up (as shown in Figure 1 (a); Shah et al. (2019)), a procedure introduced by Knapp et al. (1989, 1993) and used in many other experiments (e.g. Yao et al. (2010); Xiong et al. (2013); Hu et al. (2013)). For such scans, simulations of the ion population predict a negligible DR depletion of the Fe XVII population (see Section 4).

Every 5 s the ion inventory of the trap was dumped and regenerated to avoid contamination by W and Ba ions, which take typically a few minutes to accumulate. FLASH-EBIT uses superconductive coils inducing a magnetic field up to 6 T (Epp et al. 2010) that strongly compresses the electron beam. This beam efficiently produces ions up to the highest charge state allowed by the ionization threshold, in this case Ne-like Fe XVII. The residual pressure at the trap center stays below 10^{-12} mbar, making charge exchange (CX) with residual gas negligible. Therefore, a high-purity sample of Fe XVII ions was prepared (Shah et al. 2019). The beam current was adjusted according to \( n_e \propto E_e / \sqrt{E} \) to keep the electronic density \( n_e \) constant, having a value of 20 mA at the breeding energy. The measured electron energy spread was \( \sim 5 \) eV.

2.2. PolarX-EBIT Measurements

The new measurements used PolarX-EBIT, operating at PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg. It uses an off-axis electron gun and a magnetic field at the trap up to 0.86 T (Micke et al. 2018) produced by an assembly of permanent magnets. It operates at room temperature and had at the time of these measurements a rather poor vacuum \((10^{-8} \) mbar\), which could increase the recombination from Ne-like to Na-like ions through the CX process. As observed in Section 4, the presence of Na-like ions is not significant. PolarX-EBIT was also run at low beam current, in the present case 2 mA, and thus reached a lower \((3.5 \text{ eV FWHM at } 400 \text{ eV})\) electron energy spread than FLASH-EBIT. The measurement scheme is different (see Figure 1 (b)): here, the electron beam varies according to a square-wave scan, instead of a sawtooth scan. A breeding time of 0.4 s at 1 keV is sufficient to reach Fe XVII population equilibrium, according to both prospective measurements and simulations. The probe energy was maintained for 1 s and varied slowly (in minutes) between 300 and 500 eV. The electron energy was changed between breeding (constant) and probing values (slowly scanned) by means of a fast (tens of nanoseconds) high-voltage switch. The time evolution of the X-ray spectrum can thus be observed, in direct dependence on the evolution of the population of different charge states.

3. CALCULATIONS

DR is a resonant process involving two steps. At first, a di-electronic capture of a free electron into an initial ionic state \( i \) excites a bound electron and forms a doubly excited (or intermediate) state \( d \). Then, this state may radiatively decay into a final state \( f \), thereby completing the DR process. Following our previous works (Amaro et al. 2017; Shah et al. 2018; Shah et al. 2019), we calculated cross sections and resonant strengths in the isolated resonance approximation, i.e., no quantum interference between DR resonances (Pindzola et al. 1992), or with nonresonant recombination channels was considered (Zatsarinny et al. 2006; González Martínez et al. 2005; Tu et al. 2015, 2016). This contribution only influences weak resonances as been previously shown in Pindzola et al. (1992) and Zatsarinny et al. (2006). In this approximation, the DR strength is given by

\[
S_{df}^{DR} = \int_0^\infty \sigma_{df}^{DR}(E_e)dE_e
\]

\[
= \frac{\pi^2 \hbar^3 g_d g_{id}}{m_e E_{id} 2g_f \sum_{d'} A_{d'd}^i A_{df}^f + \sum_{f'} A_{d'f'}^f}
\]

(2)

where \( \sigma_{df}^{DR}(E_e) \) is the DR cross section as a function of the free-electron kinetic energy \( E_e \). \( E_{id}^{\text{free}} \) is the resonant energy of the electron–ion recombination between states \( i \) and \( d \), with respective statistical weights \( g_i \) and \( g_d \), and \( m_e \) is the electron mass. The autoionization rate \( A_{d}^i \) and radiative rate \( A_{df}^{\text{frac}} \) were calculated with both FAC and MCDF methods.
The details of the FAC calculation are given in Shah et al. (2019). FAC (Gu 2008) provides atomic radial wave functions and respective eigenvalues obtained in a configuration interaction method with orbitals from a modified electron–electron central potential. This code uses the distorted–wave Born approximation for calculating the autoionization rates. Beyond the standard configuration interaction module of FAC, which we employed for the initial calculations shown in Figure 4, we used the many-body perturbation theory (MBPT) option of FAC (Gu et al. 2006) for the prediction of energies and rates in the final detailed comparisons.

Calculations of the energies for the initial, intermediate, and final states as well as their respective transition and autoionization rates were also obtained with the Multiconfiguration Dirac–Fock General Matrix Elements (MCDFGME) code (version 2008) of Desclaux and Indelicato (Desclaux 1975; Indelicato et al. 1987; Indelicato & Desclaux 1990; Desclaux & Indelicato 2008). Details of the method, including the Hamiltonian and the variational processes employed for retrieving wave functions, can be found in Desclaux (1993) and Indelicato (1995). In the present calculations, the electronic correlation was restricted to mixing all states of a given \( j \) within an intermediate coupling (IC) scheme. Autoionization rates were evaluated using Fano’s single-channel discrete–continuous expansion, which allows for non-orthogonal basis sets between the initial and final states (see Howat et al. (1978) for details). Figure 2 shows our calculations of DR resonant strengths obtained using FAC and the MCDF method, as well as a comparison with Nilsen (1989) values. Note that only DR resonant strengths and the corresponding photon energies are given in Nilsen (1989). Thus, for comparing the respective resonant strengths in Figure 2 with our data, we inferred the corre-
sponding resonant energies used in that work by subtracting the photon energies the binding energy of the recombined electron in the final state. Here, the FAC-MBPT values of the binding energies were used.

Additionally, most LMM DR resonances decay through only one strong radiative channel (2p^33l3d → 2p^63l; see Figure 2(a)). We predicted with FAC the main spectral features that can be experimentally resolved in both EBITs. We found eight spectral lines that have either a single resonant contribution, like s_1, or a blend of resonances, such as p_1 or d_1. Note that in our line nomenclature we use the l of the 3l spectator electron for labeling. The observed line energies and strengths were compared with all theoretical predictions and available literature. Details are given in Appendix 6.

For spectral modeling, DR rate coefficients are convenient parameters. They can be obtained by integrating the corresponding DR resonance strengths over a Maxwellian velocity distribution of the electrons (Gu 2003),

$$\sigma_{if}^{DR} = \frac{m_e}{\sqrt{2\pi}h} \left( \frac{4E_e}{K_0 T_e} \right)^{3/2} a_0^3 \sum_d E_d \sigma_{if}^{DR} e^{-\frac{E_d}{kT_e}}, \quad (3)$$

where $E_e$ is the Rydberg constant in energy units, $a_0$ is the Bohr radius, $K_0$ is the Boltzmann constant, and $T_e$ is the electron temperature. A comparison between the present rate coefficients and those available in the OPEN-ADAS database is shown in Section 5.1.

4. SIMULATIONS OF THE CHARGE-STATE DISTRIBUTION

To measure DR resonant strengths for a given ionic species, it is necessary to know the charge-state distribution of the ions trapped in the EBIT. This is mostly determined by the following charge-changing processes: collisional ionization (CI), radiative recombination (RR), DR and CX. Their competition, depending on the measurement conditions and methods, determines the overall charge-state distribution. Here, we simulate them following the work of Penetrante et al. (1991) for computing the time evolution of the ion population in the different charge states in an EBIT by using $Z + 1$ steady-state rate equations:

$$\frac{dN_q}{dt} = n_e v_e \left[ N_{q-1} \sigma_{q-1}^{CT} + N_{q+1} (\sigma_{q+1}^{RR} + \sigma_{q+1}^{DR}) - N_q \sigma_{q}^{CT} - N_q (\sigma_{q}^{RR} + \sigma_{q}^{DR}) \right] - N_0 \sigma_{q}^{CX} v_q + N_0 N_{q+1} \sigma_{q+1}^{CX} v_{q+1}. \quad (4)$$

Here, $N_q$ denotes the population of charge states $q$, $n_e$ the electron density, $v_e$ the free-electron velocity, $\sigma$ the cross section associated with a specific atomic process, and $v_q$ the mean (Maxwellian) velocity of an ion with charge $q$. The RR total cross sections for Mg-like, Na-like, and Ne-like Fe ions under the present experimental conditions were obtained using FAC, taking into account the principal quantum numbers up to $n = 15$. For other Fe charge states, we used the analytical equation of Kim & Pratt (1983) to obtain RR cross sections. CI cross sections from the measurements performed at the TSR (Linkemann et al. 1995; Hahn et al. 2013; Bernardt et al. 2014) for Mg-like, Na-like, and Ne-like Fe ions were also used. These included, apart from the usual direct CI channel, resonant ionization processes, such as excitation and subsequent autoionization, which became strong starting from the collision excitation threshold (∼750 eV). For the remaining charge states, CI cross sections were estimated using the Lotz formula (Lotz 1968). As for the CX cross sections used in our simulations, we applied the analytical expression from Janev et al. (1983) to obtain them. However, for the more abundant charge states of Ne-like, Na-like, and Mg-like Fe, we used CX cross sections obtained using the multichannel Landau–Zener method as implemented in FAC. An ion temperature of ∼60 eV for the CX cross sections was assumed, based on the previous measurement by Schnorr et al. (2013) at FLASH-EBIT for Al-like Fe. The CX rate is proportional to the residual gas density within the trap region. Thus, by reducing the flow of the iron pentacarbonyl molecular beam in our experiment, we could enhance the population of Fe in higher charge states.

For these experiments, it is very important to choose the ratio of ionization time to recombination time appropriately to the simulation parameters. DR is a very strong resonant process; within the resonant width it has cross sections orders of magnitude higher than those of other collisional processes. This means that for our measurement scheme the Ne-like population in the trap should not be significantly depleted toward lower charge states by the required electron beam energy across the DR resonances. Therefore, we performed simulations for quantifying this depletion. We calculated the corresponding DR rates for Mg-like, Na-like, and Ne-like Fe ions using FAC. The principal quantum numbers of the recombined state up to $n = 30$ for Ne-like Fe and up to $n = 10$ for all other relevant ions were taken into account in our calculations, as well as radiative cascades for all relevant atomic processes. With these calculations we then generated synthetic X-ray emission spectra. Furthermore, our charge balance simulations were restricted to electron densities below $10^{13}$ cm$^{-3}$, the relevant range for EBIT plasmas. At values higher than those of our simulations, we note that the effect of DR suppression has to be taken into account (see Nikolić et al. (2013, 2018) and references therein).

4.1. FLASH-EBIT: Simulated Charge-state Distributions

Using Equation 4 and the scanning parameters presented in Figure 1, we simulated the time evolution of the charge-state distribution during the upward and downward electron beam energy scans in our FLASH-EBIT measurements (Shah et al. 2013).
Figure 3. (a) Spectra observed at FLASH-EBIT by scanning upward and downward the electron beam energy (see Figure 1(a) for the timing pattern). Simulations of Fe charge-state distributions as a function of the electron beam energy for effective electron densities of (b) $n_e = 2.8 \times 10^{12}$ cm$^{-3}$ ($I_e = 20$ mA) and (c) $n_e = 2.8 \times 10^{10}$ cm$^{-3}$ ($I_e = 0.2$ mA). The simulations were performed for an electron beam radius of 30 µm. (d) Experimental X-ray intensity ratio between downward and upward scans compared with simulated X-ray intensity ratios for different effective electron densities.

First, we investigated the effect of the electron beam density on the Ne-like, Na-like, and Mg-like Fe trapped-ion populations. Panel (b) of Figure 3 shows an extreme case of electron densities of $n_e \sim 10^{12}$ cm$^{-3}$, where the Ne-like population is drastically depleted into the Na-like and Mg-like ones due to strong DR resonances. In contrast, at $n_e \sim 10^{10}$ cm$^{-3}$, this effect is found to be negligible (panel (c)). In panel (d) of Figure 3, we display the experimental ratio between the fast upward and downward energy scans, which shows a negligible effect of the scanning direction on Fe XVII ion density in the trap. This stands in contrast to the out-of-equilibrium slow DR scans, where the ion populations have enough time for the decay during the scan. In this case, the two scanning directions can show clear differences in the distribution of charge states (Shah et al. 2016). We compared our present experimental ratio with those of simulations for different electron densities and found only a negligible charge-state depletion due to LMM DR resonances at electron densities below $5 \times 10^{10}$ cm$^{-3}$.

Second, we investigated the influence of CX on the Fe XVII ion population distribution. FLASH-EBIT has a four-stage differential pumping system for injecting an atomic or molecular beam into the trap, where the ions are generated. The first two stages operate at room temperature at pressures of $\sim 8 \times 10^{-9}$ mbar. Two additional stages operate cryogenically at 45 K and 4 K, and further constrain the gas flow into the trap region. This brings the residual gas pressure well below $10^{-11}$ mbar at the trap center and tremendously reduces the CX rates. For the study of a possible influence of CX in our measurements, we simulated the ion population and generated synthetic X-ray spectra for CX rates of $0.23$ s$^{-1}$ and $0.05$ s$^{-1}$ (see Figure 4). When Fe XVI and...
Fe XV ions are produced by CX, distinct DR resonances of these ions appear at beam energies of 380 and 440 eV. Since those resonances were not observed, we conclude that under the present conditions the dominant Ne-like Fe ion population was maintained during the FLASH-EBIT measurements (Shah et al. 2019).

4.2. PolarX-EBIT: Simulated Charge-state Distributions

We also simulated the time evolution of the charge-state distribution and its effect on the observed LMM DR X-ray emission for PolarX-EBIT conditions, according to the measurement technique shown in Figure 1(b). Here we compare the measurement and simulation in Figure 5. For probing times shorter than 100 ms, we observed a dominant population of Ne-like ions with a small population of Na-like and Mg-like Fe ions. However, the observed intensities of Na-like and Mg-like LMM resonances are slightly higher than those in the FLASH-EBIT measurements (see Figure 5 and Figure 4 for the resonant energy positions). Simulations at the breeding electron beam energy of 1.2 keV used in the PolarX-EBIT measurements yielded populations of 0.92±0.04, 0.07±0.03, and 0.003±0.002 for Ne-like, Na-like, and Mg-like Fe ions, respectively. These values are consistent with a negligible CX rate of 0.47 s⁻¹, as likewise observed in the FLASH-EBIT measurements.

The uncertainties given for the ion populations were estimated based on the difference between the cross sections obtained with the analytical formula of a given process (e.g., from Kim & Pratt (1983) for the RR case) and those of FAC calculations. As for the CI rates, besides using the difference between FAC and Lotz (1968) values, we also took into account the experimental uncertainties from the CI measurements performed at the TSR (Linkemann et al. 1995; Hahn et al. 2013; Bernhardt et al. 2014) for Mg-like, Na-like, and Ne-like Fe ions. For the CX cross sections, we found relative deviations between the expression of Janev et al. (1983) and FAC as high as 40%, which is in accord with observations of Betancourt-Martínez et al. (2018). However, due to the very low CX rate, uncertainties associated with the CX cross sections and ion temperature do not significantly affect the predicted Ne-like populations.

The most intense Ne-like resonances exhibit decay times between 0.07 and 0.13 s in our experiment, while Na-like resonances (e.g., at 345, 380, and 435 eV beam energies) reach their maxima between 0.2 and 0.4 s as the Ne-like population starts to deplete. For probing times longer than 1 s, the spectra are dominated by DR emission from the Mg-like and Al-like Fe populations. We also observe a constant X-Ray emission background in our experiment, which cannot be explained by simulations under any conditions of electron density and CX rate. It might be attributed to the delayed photon emission from metastable states. However, no exponential decay of the signal was observed in the FLASH-EBIT data. Another possible source might be the electronic analog-to-digital converter (ADC) noise caused by switching between power supplies.
Finally, when considering various recombination data either from FAC or MCDF theories or from TSR measurements in the charge-state distribution simulations, we did not see any change in the final synthetic spectrum. Also, this does not change our conclusion that neither spurious charge states other than Ne-like Fe nor charge-state depletion due to DR significantly affects any of the two measurements.

5. DATA ANALYSIS AND RESULTS

Experimental spectra observed in the FLASH-EBIT, PolarX-EBIT, and TSR measurements are shown in Figure 6. In the case of PolarX-EBIT, as explained in Section 4, we have only selected the first 50 ms of data in order to avoid possible charge-state depletion due to the DR and CX processes (see Figure 5). Strong DR lines were identified in Section 3, which are clearly resolved with an excellent collision energy resolution provided by both EBITs. The TSR data have a significantly better resolution than the EBIT results. However, for our comparison we synthetically broadened the TSR spectrum to match the PolarX-EBIT spectral resolution (for a complete data set, see Schmidt et al. (2009); Shah et al. (2019)).

We calibrated the electron beam energy axis using the TSR data of the $p_1$ and $d_3$ peaks. In order to compare the resonance strengths, we first subtracted an assumed linear background from the RR continua (RR+ADC for PolarX, see Section 4.2). The observed photon intensities in both EBIT spectra were normalized to a DR resonance $d_3$ at 412 eV of electron beam energy. Details of such cross-section normalization are explained in our previous work (Shah et al. 2019). In EBITs, the unidirectional electron beam causes anisotropic and polarized X-ray emission. We observed photons at 90$^\circ$ with respect to the electron beam. We thus applied a correction factor defined as $W(90^\circ) = 3/(3 - P)$, where $P$ is the polarization for a specific radiative transition (Shah et al. 2018). The calculated polarization values were taken from Shah et al. (2019), which also agree with measurements performed by Chen et al. (2004). With this correction, we obtained the total cross sections using the $S_{\text{total}} = 4\pi f^{90^\circ}/W(90^\circ)$ relation, where $f^{90^\circ}$ is the observed DR intensity. As observed in Figure 4 (Ne-like case), there are more than $\sim$200 LMM DR resonances within the scanned electron beam energy range. As most of the features observed in Figure 6 consist of a number of blended resonances, we only provide the integrated resonance strengths. For this, we defined three energy regions: $s$, 300 eV to 335 eV; $p$, 335 eV to 380 eV; and $d$, 380 eV to 440 eV.

5.1. DR Energies and Strengths

Figure 6 shows a comparison between the experimental data and predictions by FAC, FAC-MBPT, MCDF, and Nilsen (1989). All theories except MCDF predict all experimental features. FAC, in particular, shows a systematic shift in resonance energies as compared with the observed data and other theories. Also, disagreements of MCDF predictions are clearly visible for the $s_1$, $s_2$, and $p_2$ features. DR resonances within these features show larger energy splitting in the MCDF predictions than in the FAC and FAC-MBPT ones. Moreover, a clear feature at 425 eV is not predicted by

![Figure 6](image-url)
MCDF. The reason behind this might be that the MCDFGME package (Desclaux & Indelicato 2008) used in the present work could not generate reliable Auger rates with correlation to other configurations beyond minimal coupling, which would be necessary to improve the energy centroid accuracy.

Table 1 presents experimentally inferred integrated resonant strengths for the \( s, \ p, \) and \( d \) regions. We estimated total uncertainties on the level of \( \sim 13\% \) and \( \sim 11\% \), respectively, for FLASH-EBIT and PolarX-EBIT integrated resonance strengths, mainly arising from counting statistics and cross-section normalization. For the TSR results, we used the quoted uncertainty of 20\% from the original work of Schmidt et al. (2009). By combining these three independent measurements, we obtained final values for the integrated resonant strengths \( S_{\text{exp}} \) and their respective uncertainties, found to be at the level of \( \sim 10\% \) (see Table 1). As shown in the top panel of Figure 6, FAC-MBPT shows good agreement with the inferred integrated strengths, except for region \( s \). Interestingly, all theories disagree with our inferred resonance strength for the \( s \) region. Also note that no calculations can effectively predict the resonant strength of the \( p_2 \) feature. EBIT and TSR data also disagree here; since simulations seem to exclude spurious features at this energy in EBITs, at present we do not have an explanation for this.

5.2. DR Rate Coefficients

In addition to DR integrated resonant strengths, we also inferred DR rate coefficients using Equation (3) at different plasma electron temperatures. Such rate coefficients are important for collisional-radiative models of single-temperature or multi-temperature plasmas. Table 2 lists our experimentally inferred and theoretical DR rate coefficients from \( S_{\text{exp}} \) together with those available in the OPEN-ADAS and AtomDB (Zatsarinny et al. 2004; Foster et al. 2012) databases.

To compare with OPEN-ADAS, we identified the DR rates by the respective final-state configuration of the Na-like Fe ion. The combined total rates for the \( 3s, \ 3p, \) and \( 3d \) final configurations are presented in Table 2. Since the DR rates of OPEN-ADAS include all DR LMM channels, we restricted our comparison to the temperature range \( T_\text{e} \leq 250 \text{eV} \), where the LMM channel dominates \(( \geq 95\% \) of the total decay into a given final-state configuration). Two tabulated DR rates in this temperature range \((T_\text{e} = 110.3 \text{ eV} \text{ and } 220.3 \text{ eV})\) were retrieved through a file of OPEN-ADAS, namely oizLS and oizIC, respectively, as well as nrbLS and nrbIC, given by the author N. Badnell in respective atomic couplings. According to Foster et al. (2012), the Fe XVII DR rates in the AtomDB database were taken from Zatsarinny et al. (2004), calculated using the AUTOSTRUCTURE code, and summed over all final states.

Since some minor final-state configurations are shared by the observed experimental spectral features, only the total experimental rates are presented in Table 2. Figure 7 depicts the comparison between our experiment and all available DR rates over a large temperature range. Our experimental rate coefficients agree well with the theoretical rates within \( \sim 0.2–0.8\% \) for those calculated with FAC-MBPT and within \( \sim 7–14\% \) for those calculated with MCDF methods. The DR rates taken from Nilsen (1989) are in close agreement with the FAC-MBPT calculations. The OPEN-ADAS data provided by Badnell in both LS coupling and IC depart by \( \sim 9 \) to \( 12\% \) from our experimental results, while the data provided by Zatsarinny show differences of \( \sim 6–25\% \). The total DR rates obtained with AUTOSTRUCTURE (Zatsarinny et al. 2004) (also used in the AtomDB database) display differences from our results of \( <5\% \) for the entire electron temperature range.

6. SUMMARY AND CONCLUSIONS

The DR LMM resonances for Fe XVII ions have been measured using two different EBITs and compared with results obtained at the TSR (Schmidt et al. 2009). We simulated the time-dependent charge-state distribution to rule out systematic effects due to the presence of spurious charge states and depletion of charge states due to DR, which may affect our resonant strength measurements. The LMM DR integrated strengths were extracted from all three experiments, and compared with calculations performed using FAC, FAC-MBPT, and MCDF codes. Among them, FAC-MBPT calculations show the best agreement with the experiments. We

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**Figure 7.** Experimental and theoretical DR rate coefficients obtained with FAC-MBPT and MCDF and by Nilsen (1989) and Zatsarinny et al. (2004) (AUTOSTRUCTURE), as well as tabulated values for two temperatures from adf09 files of OPEN-ADAS, namely oizLS, oizIC, nrbLS, and nrbIC.
Table 1. Experimental Integrated Resonant Strengths ($10^{-20}$cm$^2$eV) Compared to Values Obtained with FAC and MCDF (This Work) and Those Reported by Nilsen (1989).

| Label | $S_{\text{FLASH}}$ | $S_{\text{PolarX}}$ | $S_{\text{TSR}}$ | $S_{\text{EXP}}$ | $S_{\text{FAC}}$ | $S_{\text{FAC-MBPT}}$ | $S_{\text{MCDF}}$ | Nilsen (1989) |
|-------|---------------------|----------------------|------------------|----------------|------------------|------------------|-----------------|----------------|
| s     | 80 ± 10             | 65 ± 9               | 100 ± 10         | 80 ± 6         | 104.27 (-30%)    | 97.77 (-22%)     | 62.66 (22%)     | 106.25 (-32%)   |
| p     | 210 ± 30            | 230 ± 20             | 230 ± 50         | 220 ± 20       | 201.18 (15%)     | 198.34 (11%)     | 202.89 (25%)    | 174.30 (20%)    |
| d     | 300 ± 40            | 280 ± 30             | 330 ± 70         | 290 ± 20       | 271.76 (13%)     | 283.43 (4%)      | 270.29 (25%)    | 306.67 (-5%)    |

Note. The listed experimental cross sections were calibrated with the FAC-MBPT theoretical value of the d$_3$ feature. Round brackets: Relative difference in percent between measured and theoretical resonant strengths, where each measurement was independently calibrated with the d$_3$ value from respective theories. The labels s, p and d correspond to regions of 300 eV to 340 eV, 340 eV to 380 eV, and 380 eV to 420 eV, respectively.

Table 2. Experimental DR Rate Coefficients ($\times 10^{-13}$cm$^3$s$^{-1}$) for a Few Electron Temperatures $T_e$ (eV) Compared to Values Obtained with FAC-MBPT and MCDF and by Nilsen (1989) and by Zatsarinny et al. (2004).

| Label | $T_e$ | Exp. | OPEN-ADAS | FAC-MBPT | MCDF | Nilsen (1989) | Zatsarinny et al. (2004) |
|-------|-------|------|-----------|----------|------|---------------|--------------------------|
|       |       |      | oizLS     | oizIC    | nrbLS | nrbIC         |                          |
| 3s    | 110.3 | ...  | 10.9      | 9.24     | 10.6  | 7.04          | 8.96                     | 6.40                      | 9.28                      |
| 220.3 | ...   | 17.4 | 15.0      | 11.9     | ...   | ...           | 13.7                     | 10.3                      | 14.4                      |
| 300   | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| 2000  | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| 3p    | 110.3 | ...  | 20.1      | 20.4     | 16.8  | 17.2          | 18.8                     | 17.1                      | 16.5                      |
| 220.3 | ...   | 40.3 | 42.2      | 36.4     | 38.9  | ...           | 33.0                     | 30.9                      | 29.5                      |
| 300   | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| 2000  | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| 3d    | 110.3 | ...  | 18.9      | 21.2     | 15.9  | 16.9          | 19.2                     | 16.8                      | 20.6                      |
| 220.3 | ...   | 46.2 | 52.6      | 41.4     | 45.4  | ...           | 40.7                     | 36.6                      | 43.8                      |
| 300   | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| 2000  | ...   | ...  | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      |
| total | 110.3 | 47 ± 3 | 49.9      | 50.9     | 43.3  | 41.2          | 46.9                     | 40.3                      | 46.4                      | 46.6                      |
|       |       |       | (-6.2%)   | (-8.2%)  | (7.9%) | (12%)         | (0.2%)                   | (14%)                     | (1.3%)                    | (0.8%)                    |
| 220.3 | 88 ± 4 | ... | 103.9     | 109.8    | 95.2  | 96.2          | 87.4                     | 77.7                      | 87.6                      | 91.0                      |
|       |       |       | (-18%)    | (-25%)   | (-8.2%)| (-9.3%)       | (0.7%)                   | (12%)                     | (0.4%)                    | (-3.5%)                   |
| 300   | 87 ± 4 | ... | ...       | ...      | ...   | ...           | 86.0                     | 77.2                      | 86.6                      | 90.3                      |
|       |       |       | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      | ...                      |
| 2000  | 14.5 ± 0.7 | ... | ...       | ...      | ...   | ...           | 14.5                     | 13.2                      | 14.7                      | 15.3                      |
|       |       |       | ...       | ...      | ...   | ...           | ...                      | ...                      | ...                      | ...                      |

Notes. The first label indicates the orbital of the decoupled electron in the final state after DR emission. Labels oizLS, oizIC, nrbLS and nrbIC refer to data files available at a df09 of OPEN-ADAS.

* Only total DR LMM rates are provided.

also derived from our experimental data LMM DR rate coefficients for several temperatures. Our experimental rates show good agreement with rates obtained from Nilsen (1989) and FAC-MBPT, while rates available in the OPEN-ADAS and AtomDB databases, which are frequently used for the analysis of astrophysical spectra, show departures from our experimentally inferred values. These differences highlight how crucial laboratory measurements are for testing different spectral models. This is important not only from the perspective of upcoming X-ray satellite missions XRISM (Tashiro et al. 2018) and Athena (Barret et al. 2016), which will soon provide high-resolution spectra using X-ray microcalorimeters (Durkin et al. 2019), but also for interpreting available high-resolution spectra from the operating Chandra and XMM-Newton observatories (Gu et al. 2020) needed for reliable plasma diagnostics (Beiersdorfer et al. 2014, 2018).

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APPENDIX

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DR CALCULATIONS FOR FE XVII

Table 3 contains the resonant energies and strengths for the main spectral features that are benchmarked in this work. The emitted wavelengths of the decay channels are listed in Table 4 with additional data provided by Nilsen (1989) and Beiersdorfer et al. (2014).

The complete set of resonant energies, strengths, and emitted wavelengths calculated within this work (FAC, FAC-MBPT, and MCDF methods) is available online as machine-readable tables. These data can be used to make Figure 2 as well as to produce the synthetic spectra shown in Figure 6.
### Table 3. Theoretical Values of the Peak Resonant Energies $E$ (eV) and Strengths $S$ (10$^{-20}$cm$^2$eV) Obtained in This Work with FAC, FAC-MBPT, and MCDF.

| Label | Intermediate State | Final State | $E_{FAC}$ | $E_{MBPT}$ | $E_{MCDF}$ | $S_{FAC}$ | $S_{MBPT}$ | $S_{MCDF}$ |
|-------|---------------------|-------------|-----------|------------|------------|-----------|------------|------------|
| $s_1$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3s$_{1/2}^1$,3d$_{s1}^1$) | 4D$_{1/2}$ | 3s$_{1/2}^1$5s$_{1/2}^1$ | 313.06 | 310.23 | 313.08 | 6.04 | 6.42 | 2.74 |
| $s_2$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3s$_{1/2}^1$,3d$_{s1}^1$) | 2D$_{3/2}$ | 3s$_{1/2}^1$5s$_{1/2}^1$ | 325.70 | 322.21 | 321.98 | 31.91 | 29.54 | 7.34 |
| $p_1$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3p$_{1/2}^1$,3d$_{s1}^1$) | 4F$_{3/2}$ | 3p$_{1/2}^1$2p$_{1/2}^1$ | 353.65 | 355.05 | 352.28 | 1.06 | 9.70 | 0.16 |
| $p_2$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3p$_{1/2}^1$,3d$_{s1}^1$) | 2P$_{1/2}$ | 3p$_{1/2}^1$2p$_{1/2}^1$ | 364.85 | 361.80 | 364.06 | 10.77 | 11.87 | 19.61 |
| $d_1$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3d$_{s1}^1$) | 4G$_{5/2}$ | 3d$_{5/2}^1$D$_{1/2}^1$ | 396.39 | 393.3 | 396.73 | 9.42 | 11.46 | 11.37 |
| $d_2$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3d$_{s1}^1$) | 2F$_{5/2}$ | 3d$_{5/2}^1$D$_{1/2}^1$ | 405.22 | 401.98 | 403.14 | 41.48 | 23.62 | 35.91 |
| $d_3$ | (2p$_{1/2}^1$2p$_{3/2}^1$,3d$_{s1}^1$) | 2F$_{5/2}$ | 3d$_{5/2}^1$D$_{1/2}^1$ | 411.90 | 410.07 | 401.07 | 60.63 | 58.13 | 52.73 |

Note. The resonant and final states are given in jj and LSJ notations.

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Table 4. Theoretical Values of Emitted Wavelengths (Å) Obtained in This Work with FAC, FAC-MBPT, and MCDF.

| Label | Intermediate State | Final State | $\lambda_{\text{FAC}}$ | $\lambda_{\text{FAC-MBPT}}$ | $\lambda_{\text{MCDF}}$ | Nilsen (1989) | Beiersdorfer et al. (2014) |
|-------|---------------------|-------------|-----------------|------------------|-----------------|----------------|-------------------|
| $s_1$ | $[(2p_{1/2}^3/2p_{1/2}^3/2s_{1/2})_{3/2}3d_{3/2}^1l_{1/2}]$ | $^4D_{3/2}$ | 15.47 | 15.52 | 15.52 | 15.49 |
| $s_2$ | $[(2p_{1/2}^3/2p_{1/2}^3/2s_{1/2})_{3/2}3d_{3/2}^1l_{1/2}]$ | $^2P_{1/2}$ | 15.06 | 15.13 | 15.17 | 15.12 | 15.11 |
| $d_1$ | $[(2p_{1/2}^3/2p_{1/2}^3/2s_{1/2})_{3/2}3d_{3/2}^1l_{1/2}]$ | $^4F_{3/2}$ | 15.35 | 15.32 | 15.37 | 15.40 | 15.30 |
| $d_2$ | $[(2p_{1/2}^3/2p_{1/2}^3/2s_{1/2})_{3/2}3d_{3/2}^1l_{1/2}]$ | $^2P_{1/2}$ | 15.19 | 15.24 | ... | 15.23 | 15.24 |
| $d_3$ | $[(2p_{1/2}^3/2p_{1/2}^3/2s_{1/2})_{3/2}3d_{3/2}^1l_{1/2}]$ | $^2D_{9/2}$ | 15.53 | 15.47 | 15.54 | 15.50 |

Notes. The resonant and final states are given in $j$-$j$ and LSJ notations. The respective data provided by Nilsen (1989) and by Beiersdorfer et al. (2014) are also listed for comparison.
