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DIELECTRONIC RECOMBINATION OF Fe XV FORMING Fe XIV: LABORATORY MEASUREMENTS AND THEORETICAL CALCULATIONS

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ABSTRACT

We have measured resonance strengths and energies for dielectronic recombination (DR) of Mg-like Fe XV forming Al-like Fe XIV via $N = 3 \rightarrow N' = 3$ core excitations in the electron-ion collision energy range 0–45 eV. All measurements were carried out using the heavy-ion test storage ring at the Max Planck Institute for Nuclear Physics in Heidelberg, Germany. We have also carried out new multiconfiguration Breit-Pauli (MCBP) calculations using the AUTOSTRUCTURE code. For electron-ion collision energies $\lesssim$25 eV we find poor agreement between our experimental and theoretical resonance energies and strengths. From 25 to 42 eV we find good agreement between the two for resonance energies. But in this energy range the theoretical resonance strengths are $\approx$31% larger than the experimental results. This is larger than our estimated total experimental uncertainty in this energy range of ±26% (at a 90% confidence level). Above 42 eV the difference in the shape between the calculated and measured $3s3p(^1P_1)nl$ DR series limit we attribute partly to the nl dependence of the detection probabilities of high Rydberg states in the experiment. We have used our measurements, supplemented by our AUTOSTRUCTURE calculations, to produce a Maxwellian-averaged $3 \rightarrow 3$ DR rate coefficient for Fe XV forming Fe XIV. The resulting rate coefficient is estimated to be accurate to better than ±29% (at a 90% confidence level) for $k_B T_e \geq 1$ eV. At temperatures of $k_B T_e \approx 2.5$–15 eV, where Fe XV is predicted to form in photoionized plasmas, significant discrepancies are found between our experimentally derived rate coefficient and previously published theoretical results. Our new MCBP plasma rate coefficient is 19%–28% smaller than our experimental results over this temperature range.

Subject headings: atomic data — atomic processes — galaxies: active — galaxies: nuclei — plasmas — X-rays: galaxies

1. INTRODUCTION

Recent *Chandra* and *XMM Newton* X-ray observations of active galactic nuclei (AGNs) have detected a new absorption feature in the 15–17 Å wavelength range. This has been identified as an unresolved transition array (UTA) due mainly to $2p$–$3d$ inner shell absorption in iron ions with an open M-shell (Fe I–XVI). UTAs have been observed in IRAS 13349+2438 (Sako et al. 2001), Mrk 509 (Pounds et al. 2001), NGC 3783 (Blustin et al. 2002; Kaspi et al. 2002; Behar et al. 2003), NGC 5548 (Steenbrugge et al. 2003), MR 2251−178 (Kaspi et al. 2004), I Zw 1 (Gallo et al. 2004), NGC 4051 (Pounds et al. 2004), and NGC 985 (Krongold et al. 2005).

Based on atomic structure calculations and photoabsorbtion modeling, Behar et al. (2001) have shown that the shape, central wavelength, and equivalent width of the UTA can be used to diagnose the properties of AGN warm absorbers. However, models which fit well absorption features from second- and third-row elements cannot reproduce correctly the observed UTAs due to the fourth-row element iron. The models appear to predict too high an ionization level for iron. Netzer et al. (2003) attributed this discrepancy to an underestimate of the low-temperature dielectronic recombination (DR) rate coefficients for Fe M-shell ions. To investigate this possibility Netzer (2004) and Kraemer et al. (2004) arbitrarily increased the low-temperature Fe M-shell DR rate coefficients. Their model results obtained with the modified DR rate coefficients support the hypothesis of Netzer et al. (2003). New calculations by Badnell (2006a) using a state-of-the-art theoretical method discussed in § 5 further support the hypothesis of Netzer et al. (2003).

Astrophysical models currently use the DR data for Fe M-shell ions recommended by Arnaud & Raymond (1992). These data are based on theoretical DR calculations by Jacobs et al. (1977) and Hahn (1989). The emphasis of this early theoretical work was on producing data for modeling collisional ionization equilibrium (sometimes also called coronal equilibrium). Under these

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conditions an ion forms at a temperature about an order of magnitude higher than the temperature where it forms in photoionized plasmas (Kallman & Bautista 2001). The use of the Arnaud & Raymond (1992) recommended DR data for modeling photoionized plasmas is thus questionable. Benchmarking by experiment is highly desirable.

Reliable experimentally derived low-temperature DR rate coefficients of M-shell iron ions are just now becoming available. Until recently, the only published Fe M-shell DR measurements were for Na-like Fe XVI (Linkemann et al. 1995; Müller 1999; here and throughout we use the convention of identifying the recombination process by the initial charge state of the ion). The Na-like measurements were followed up with modern theoretical calculations (Gorczyca & Badnell 1996; Gu 2003; Altun et al. 2006). Additional M-shell experimental work also exists for Na-like Ni XVIII (Fogle et al. 2003) and Ar-like Sc IV and Ti V (Schippers et al. 1998, 2002). We have undertaken the measurement of low-temperature DR for other Fe M-shell ions. Our results for Al-like Fe XIV are presented in Schmidt et al. (2006) and Badnell (2006b). The present paper is a continuation of this research.

DR is a two-step recombination process that begins when a free electron approaches an ion, collisionally excites a bound electron of the ion, and is simultaneously captured into a Rydberg level n. The electron excitation can be labeled $Nl_j \rightarrow N'l'_{j'}$, where N is the principal quantum number of the core electron, l is its orbital angular momentum, and j is its total angular momentum. The intermediate state, formed by simultaneous excitation and capture, may autoionize. The DR process is complete when the intermediate state emits a photon which reduces the total energy of the recombined ion to below its ionization limit.

In this paper we present experimental and theoretical results for $\Delta N = N' - N = 0$ DR of Mg-like Fe XV forming Al-like Fe XIV. In particular, we have studied $3 \rightarrow 3$ DR via the resonances

$$\mathrm{Fe}^{14+}\left(3s^2\left[{}^1\mathrm{S}_0\right]\right) + e^- \rightarrow \begin{cases} \mathrm{Fe}^{13+}\left(3s3p\left[{}^3P^o_{0,1,2};\, {}^1P_1\right]nl\right) \\ \mathrm{Fe}^{13+}\left(3s3d\left[{}^3D_{1,2,3};\, {}^1D_2\right]nl\right) \\ \mathrm{Fe}^{13+}\left(3p^2\left[{}^3P_{0,1,2};\, {}^1D_2;\, {}^1S_0\right]nl\right) \\ \mathrm{Fe}^{13+}\left(3p3d\left[{}^3D^o_{1,2,3};\, {}^3F^o_{2,3,4};\, {}^3P^o_{0,1,2};\, {}^1P^o_1;\, {}^1D^o_2;\, {}^1F^o_3\right]nl\right) \\ \mathrm{Fe}^{13+}\left(3d^2\left[{}^3P_{0,1,2};\, {}^3F_{2,3,4};\, {}^1D_2;\, {}^1G_4;\, {}^1S_0\right]nl\right). \end{cases} \tag{1}$$

Possible contributions due to $3s3p\ {}^3P$ metastable parent ions will be discussed below. Table 1 lists the excitation energies for the relevant Fe XV levels, relative to the ground state, that have been considered in our theoretical calculations. In our studies we have carried out measurements for electron-ion center-of-mass collision energies E_{cm} between 0 and 45 eV.

Our work is motivated by the "formation zone" of Fe M-shell ions in photoionized gas. This zone may be defined as the temperature range where the fractional abundance of a given ion is greater than 10% of its peak value (Schippers et al. 2004). We adopt this definition for this paper. Savin et al. (1997, 1999, 2002a, 2002b, 2006) defined this zone as the temperature range where the fractional abundance is greater than 10% of the total elemental abundance. This is narrower than the Schippers et al. (2004) definition. For Fe XV the wider definition corresponds to a $k_{\mathrm{B}}T_e \approx 2.5$–15 eV (Kallman & Bautista 2001). It should be kept in mind that this temperature range depends on the accuracy of the underlying atomic data used to calculate the ionization balance and also on the shape of the ionizing spectrum, the metallicity of the gas, and any additional heating or cooling mechanisms.

TABLE 1

Energy Levels for the $n = 3$ Shell of Fe XV Relative to the Ground State

Level	Energy[a] (eV)
$3s3p(^3P^o_0)$	28.9927
$3s3p(^3P^o_1)$	29.7141
$3s3p(^3P^o_2)$	31.4697
$3s3p(^1P^o_1)$	43.6314
$3p^2(^3P_0)$	68.7522
$3p^2(^1D_2)$	69.3816
$3p^2(^3P_1)$	70.0017
$3p^2(^3P_2)$	72.1344
$3p^2(^1S_0)$	81.7833
$3s3d(^3D_1)$	84.1570
$3s3d(^3D_2)$	84.2826
$3s3d(^3D_3)$	84.4848
$3s3d(^1D_2)$	94.4875
$3p3d(^3F^o_2)$	115.087
$3p3d(^3F^o_3)$	116.313
$3p3d(^3F^o_4)$	117.743
$3p3d(^1D^o_2)$	117.601
$3p3d(^3D^o_1)$	121.860
$3p3d(^3D^o_3)$	123.346
$3p3d(^3D^o_2)$	123.565
$3p3d(^3P^o_2)$	121.940
$3p3d(^3P^o_0)$	123.474
$3p3d(^3P^o_1)$	123.518
$3p3d(^1F^o_3)$	131.7351
$3p3d(^1P^o_1)$	133.2690
$3d^2(^3\mathrm{F}_2)$	169.8994
$3d^2(^3\mathrm{F}_3)$	170.1106
$3d^2(^3\mathrm{F}_4)$	170.3612
$3d^2(^1D_2)$	173.8992
$3d^2(^1G_4)$	174.4529
$3d^2(^3P_0)$	174.2613[b]
$3d^2(^3P_1)$	174.3433[b]
$3d^2(^3P_2)$	174.5416
$3d^2(^1S_0)$	184.3712

[a] Values from Ralchenko et al. (2006) unless otherwise noted.

[b] Value from Churilov et al. (1989).

The paper is organized as follows. The experimental arrangement for our measurements is described in § 2. Possible contamination of our parent ion beam by metastable ions is discussed in § 3. Our laboratory results are presented in § 4. In this section the experimentally derived DR rate coefficient for a Maxwellian plasma is provided as well. Theoretical calculations which have been carried out for comparison with our experimental results are discussed in § 5. Comparison between the experimental and theoretical results is presented in § 6. A summary of our results is given in § 7.

2. EXPERIMENTAL TECHNIQUE

DR measurements were carried out at the heavy ion test storage ring (TSR) of the Max Planck Institute for Nuclear Physics (MPI-K) in Heidelberg. A merged-beams technique was used. A beam of $^{56}\mathrm{Fe}^{14+}$ with an energy of 156 MeV was provided by the MPI-K accelerator facility. Ions were injected into the ring, and their energy spread reduced using electron cooling (Kilgus et al. 1990). Typical waiting times after injection and before measurement were ≈1 s. Mean stored ion currents were ≈10 μA. Details of the experimental setup have been given elsewhere (Kilgus et al. 1992; Lampert et al. 1996; Schippers et al. 1998, 2000, 2001).

Recently a second electron beam has been installed at the TSR (Sprenger et al. 2004; Kreckel et al. 2005). This allows one to use the first electron beam for continuous cooling of the stored ions and to use the second electron beam as a target for the stored ions. In this way a low velocity and spatial spread of the ions can be maintained throughout the course of a DR measurement. The combination of an electron cooler and an electron target can be used to scan energy-dependent electron-ion collision cross sections with exceptional energy resolution. In comparison to the electron cooler, the electron source and the electron beam are considerably smaller, and additional procedures, such as the stabilization of the beam positions during energy scans and electron beam profile measurements, are required to control the absolute luminosity product between the ion and electron beam on the same precise level as reached at the cooler. The target electron beam current was ≈3 mA. The beam was adiabatically expanded from a diameter of 1.6 mm at the cathode to 7.5 mm in the interaction region using an expansion factor of 22. This was achieved by lowering the guiding magnetic field from 1.28 T at the cathode to 0.058 T in the interaction region, thus reducing the transverse temperature to approximately 6 meV. The relative electron-ion collision energy can be precisely controlled, and the recombination signal measured as a function of this energy. We estimate that the uncertainty of our scale for $E_{\rm cm}$ is $\lesssim 0.5\%$.

The electrons are merged and demerged with the ion beam using toroidal magnets. After demerging, the primary and recombined ion beams pass through two correction dipole magnets and continue into a bending dipole magnet. Recombined ions are bent less strongly than the primary ion beam, and they are directed onto a particle detector used in single-particle counting mode. Some of the recombined ions can be field-ionized by motional electric fields between the electron target and the detector and thus are not detected. Here we assumed a sharp field ionization cutoff and estimated for Fe xv that only electrons captured into $n_{\rm max} \lesssim 80$ are detected by our experimental arrangement.

The experimental energy distribution can be described as a flattened Maxwellian distribution. It is characterized by the transversal and longitudinal temperatures $T_\perp$ and $T_\parallel$, respectively. The experimental energy spread depends on the electron-ion collision energy and can be approximated according to the formula $\Delta E = \{[\ln(2) k_{\rm B} T_\perp]^2 + 16 \ln(2) E_{\rm cm} k_{\rm B} T_\parallel\}^{1/2}$ (Pastuszka et al. 1996). For the comparison of our theoretical calculations with our experimental data, we convolute the theoretical results described in § 5 with the velocity distribution function given by Dittner et al. (1986) to simulate the experimental energy spread.

With the new combination of an electron target and an electron cooler, we obtain in the present experiment electron temperatures of $k_{\rm B} T_\perp \approx 6$ meV and $k_{\rm B} T_\parallel \approx 0.05$ meV. In order to verify the absolute calibration of the absolute rate coefficient scale, we also performed a measurement with the electron cooler using the previous standard method (Kilgus et al. 1992; Lampert et al. 1996). We find consistent rate coefficients and spectral shapes, while the electron temperatures were larger by a factor of about 2 with the electron cooler alone. Moreover, because of the large density of resonances found in certain regions of the Fe xv DR spectrum, the determination of the background level for the DR signal was considerably more reliable in the higher resolution electron target data than in the lower resolution cooler data. Hence, we performed the detailed analysis presented below on the electron target data only.

Details of the experimental and data reduction procedure are given in Schippers et al. (2001, 2004) and Savin et al. (2003) and references therein. The baseline experimental uncertainty (systematic and statistical) of the DR measurements is estimated to be ±25% at a 90% confidence level (Lampert et al. 1996). The major sources of uncertainties include the electron beam density determination, ion current measurements, and corrections for the merging and demerging of the two beams. Additional uncertainties discussed below result in a higher total experimental uncertainty, as is explained in §§ 3 and 4. Unless stated otherwise all uncertainties in this paper are cited at an estimated 90% confidence level.

3. METASTABLE IONS

For Mg-like ions with zero nuclear spin (such as ^{56}Fe), the $1s^2 2s^2 2p^6 3s3p\ ^3P_0$ level is forbidden to decay to the ground state via a one-photon transition, and the multiphoton transition rate is negligible. Therefore, this level can be considered as having a nearly infinite lifetime (Marques et al. 1993; Brage et al. 1998). It is possible that these metastables are present in the ion beam used for the present measurements.

We estimate that the largest possible metastable $^3P_0$ fraction in our stored beam is 11%. This assumes that 100% of the initial $\rm Fe^{14+}$ ions are in ^3P_J levels and that the levels are statistically populated. We expect that the $J = 1$ and 2 levels will radiatively decay to the ground state during the ~1 s between injection and measurement. The lifetimes of the $^3P_1$ and $^3P_2$ levels are $\sim 1.4 \times 10^{-10}$ s (Marques et al. 1993) and ~0.3 s (Brage et al. 1998), respectively. These decays leave one-ninth or 11% of the stored ions in the $^3P_0$ level.

Our estimate is only slightly higher than the inferred metastable fraction for the ion beam used for DR measurements of the analogous Be-like $\rm Fe^{22+}$ (Savin et al. 2006). The Be-like system has a metastable $1s^2 2s2p\ ^3P_0$ state, and following the above logic the stored Be-like ion beam had an estimated maximum 11% $^3P_0$ fraction. Fortunately, for the Be-like measurements we were able to identify DR resonances due to the $^3P_0$ parent ion and use the ratio of the experimental to theoretical resonance strengths to infer the $^3P_0$ fraction. There we determined a metastable fraction of 7% ± 2%. A similar fraction was inferred for DR measurements with Be-like $\rm Ti^{18+}$ ions (Schippers et al. 2007).

Using theory as a guide, we have searched our Mg-like data fruitlessly for clearly identifiable DR resonances due to metastable $^3P_0$ parent ions. First, following our work in the analogous Be-like $\rm Fe^{22+}$ with its $2s2p\ ^3P_0 \to 2p^2$ core excitation channel (Savin et al. 2006), we searched for $\rm Fe^{14+}$ resonances associated with the relevant $3s3p\ ^3P_0 \to 3p^2$ core excitations. However, most of these yield only very small DR cross sections as they strongly autoionize into the $3s3p\ ^3P_{J=1,2}$ continuum channels. These are energetically open at $E_{\rm cm}$ greater than 0.713 and 2.468 eV, respectively (Table 1). Hence, above $E_{\rm cm} \approx 0.713$ eV there are no predicted significant DR resonances for metastable $\rm Fe^{14+}$ via $3s3p\ ^3P_0 \to 3p^2$ core excitations. Below this energy the agreement between theory and experiment is extremely poor (as can be seen in Fig. 1), and we are unable to assign unambiguously any DR resonance to either the ground state or metastable parent ion. Second, we searched for resonances associated with $3s3p\ ^3P_0 \to 3s3p\ ^1P_1$, $3s3p\ ^3P_0 \to 3s3p\ ^3P_1$, and $3s3p\ ^3P_0 \to 3s3p\ ^3P_2$ core excitation which are energetically possible for capture into the $n \geq 14$, 62, and 33 levels, respectively, and which may contribute to the observed resonance structures. The analogous $2s2p\ ^3P_0 \to 2s2p\ ^1P_1$ and $2s2p\ ^3P_0 \to 2s2p\ ^3P_2$ core excitations were seen for Be-like $\rm Ti^{18+}$ (Schippers et al. 2007). However, again the complexity of the Fe xv DR resonance spectrum (e.g., Fig. 1) prevented unambiguous identification for DR via any of these three core excitations. Hence, despite these two

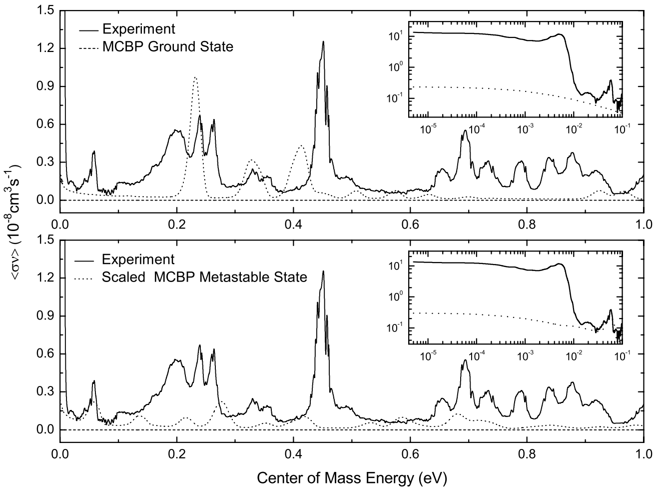

FIG. 1.—Fe xv to Fe xiv 3 → 3 DR resonance structure vs. center-of-mass energy $E_{\rm cm}$ from 0 to 1 eV. The solid curve represents the measured rate coefficient $\langle\sigma v\rangle$, which is the summed DR plus radiative recombination (RR) cross sections times the relative velocity convolved with the experimental energy spread, i.e., a merged-beam recombination rate coefficient (MBRRC). The dotted curve shows our calculated multiconfiguration Breit-Pauli (MCBP) results ($n_{\rm max} = 80$) for ground state Fe xv (*top*) and the $^3P_0$ metastable state Fe xv multiplied by a factor of 0.06 to account for the estimated 6% population in our ion beam (*bottom*). To these results we have added the convolved, nonresonant RR contribution obtained from semiclassical calculations (Schippers et al. 2001). The inset shows our results for $E_{\rm cm}$ from 5×10^{-6} to 1×10^{-1} eV.

approaches, we have been unable to directly determine the metastable fraction of our Fe^{14+} beam.

Clearly our assumption that the ^3P_J levels are statistically populated is questionable. Ion beam generation using beam foil techniques are known to produce excited levels. The subsequent cascade relaxation could potentially populate the J levels nonstatistically (Martinson & Gaupp 1974; Quinet et al. 1999). In addition the magnetic sublevels m_J can be populated nonstatistically (Martinson & Gaupp 1974), which may affect the J levels. However, our argument in the above paragraphs that the ^3P_J levels are statistically populated yields $^3P_0$ fractions of the analogous Be-like Ti^{18+} and Fe^{22+} of 11%, while our measurements found metastable fractions of ~7% for those two beams. From this we conclude either (1) that if 100% of the initial ions are in the ^3P_J levels, then the $J = 0$ level is statistically underpopulated, or (2) that the fraction of initial ions in the ^3P_J levels is less than 100% by a quantity large enough that any nonstatistical populating of the various J levels still yields only a 7% $^3P_0$ metastable fraction of the ion beam. Thus, we believe that our assumption provides a reasonable upper limit to the metastable fraction of the Fe^{14+} beam.

Based on our estimates above and the Be-like results, we have assumed that 6% ± 6% of the Fe^{14+} ions are in the $3s3p\ ^3P_0$ metastable state and the remaining fraction in the $3s^2\ ^1S_0$ ground state. Here, we treat this possible 6% systematic error as a stochastic uncertainty and add it in quadrature with the 25% uncertainty discussed above.

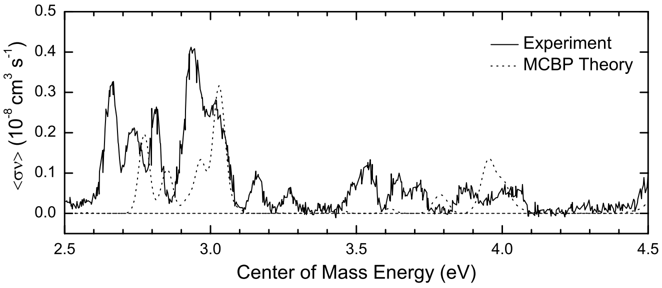

FIG. 3.—Same as Fig. 2, but for $E_{\rm cm}$ from 2.5 to 4.5 eV.

4. EXPERIMENTAL RESULTS

Our measured 3 → 3 DR resonance spectrum for Fe xv is shown in Figures 1–8. The data $\langle\sigma v\rangle$ represent the summed DR and radiative recombination (RR) cross sections times the relative velocity convolved with the energy spread of the experiment, i.e., a merged-beam recombination rate coefficient (MBRRC).

The strongest DR resonance series corresponds to $3s^2\ ^1S_0 \rightarrow 3s3p\ ^1P_1$ core excitations. Other observed features in the DR resonance spectrum are possibly due to double core excitations discussed in § 1. Trielectronic recombination (TR), as this has been named, has been observed in Be-like ions (Schnell et al. 2003a, 2003b; Fogle et al. 2005). These ions are the second-row analog to third-row Mg-like ions. However, in our data unambiguous assignment of possible candidates for the TR resonances could not be made.

Extracted resonance energies E_i and resonance strengths S_i for $E_{\rm cm} \leq 0.95$ eV are listed in Table 2 along with their fitting errors. These data were derived following the method outlined in Kilgus et al. (1992). Most of these resonances were not seen in any of the theoretical calculations for either ground state or metastable Fe^{14+}. Thus, their parentage is uncertain. The implications of this are discussed below.

Difficulties in determining the nonresonant background level of the data contributed an uncertainty to the extracted DR resonance strengths. For the strongest peaks, this was on the order of ≈10% for $E_{\rm cm} \lesssim 5$ eV and ≈3% for $E_{\rm cm} \gtrsim 5$ eV. Taking into account the 25% and 6% uncertainties discussed in §§ 2 and 3, respectively, this results in an estimated total experimental uncertainty for extracted DR resonance strengths of ±28% below ≈5 eV and ±26% above.

Because of the energy spread of the electron beam, resonances below $E_{\rm cm} \lesssim k_{\rm B}T_\perp$ cannot be resolved from the near 0 eV RR

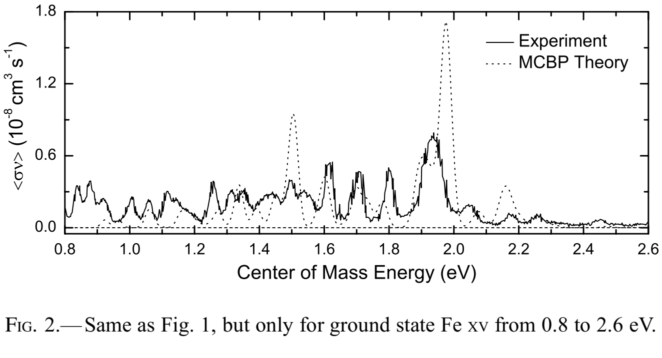

FIG. 2.—Same as Fig. 1, but only for ground state Fe xv from 0.8 to 2.6 eV.

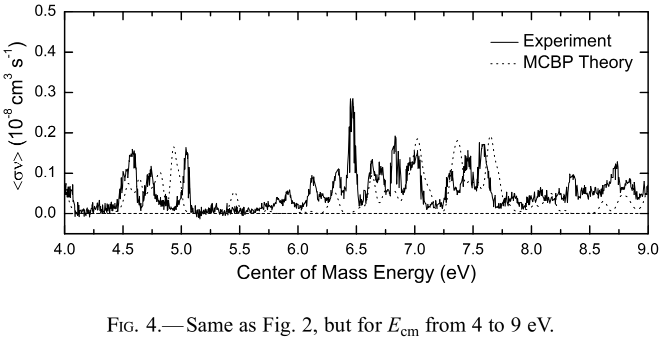

FIG. 4.—Same as Fig. 2, but for $E_{\rm cm}$ from 4 to 9 eV.

to unsubtracted metastable $^3P_0$ contributions. But these contributions are $<10\%$ at 2.5 eV, $<5\%$ at 5 eV, $<2.0\%$ at 10 eV, and $<1.4\%$ above 15 eV (hence basically insignificant). Above 15 eV the difference decreases and at 23 eV and up the agreement is within $\lesssim 10\%$ with theory initially smaller than experiment but later greater. Part of the good agreement at these higher temperatures is due to our use of theory for the unmeasured DR contribution due to states with $n > 80$.

7. SUMMARY

We have measured resonance strengths and energies for $\Delta N = 0$ DR of Mg-like Fe xv forming Al-like Fe xiv for center-of-mass collision energies $E_{\rm cm}$ from 0 to 45 eV and compared our results with new MCBP calculations. We have generated an experimentally derived plasma rate coefficient by convolving the measured MBRRC with a Maxwell-Boltzmann electron energy distribution. We have supplemented our measured MBRRC with MCBP calculations to account for unmeasured DR into states which are field-ionized before detection. The resulting plasma recombination rate coefficient has been compared to the recommended rate coefficient of Arnaud & Raymond (1992) and new calculations using a state-of-the-art MCBP theoretical method. We have considered the issues of metastable ions in our stored ion beam, enhanced recombination for collision energies near 0 eV, and field-ionization of high Rydberg states in the storage ring bending magnets.

As suggested by Netzer et al. (2003) and Kraemer et al. (2004), the present result shows that the previously available theoretical DR rate coefficients for Fe xv are much too low. Other storage ring measurements show similar differences with published recommended low-temperature DR rate coefficients for M-shell iron ions (Müller 1999; Schmidt et al. 2006). We are now in the process of carrying out DR measurements for additional Fe M-shell ions. As these data become available we recommend that these experimentally derived DR rate coefficients be incorporated into AGN spectral models in order to produce more reliable results.

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