Dielectronic Recombination (via $N = 2 \rightarrow N' = 2$ Core Excitations) and Radiative Recombination of Fe XX: Laboratory Measurements and Theoretical Calculations

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ABSTRACT

We have measured the resonance strengths and energies for dielectronic recombination (DR) of Fe XX forming Fe XIX via $N = 2 \rightarrow N' = 2$ ($\Delta N = 0$) core excitations. We have also calculated the DR resonance strengths and energies using AUTOSTRUCTURE, HULLAC, MCDF, and R-matrix methods, four different state-of-the-art theoretical techniques. On average the theoretical resonance
strengths agree to within \( \lesssim 10\% \) with experiment. The AUTOSTRUCTURE, MCDF and R-matrix results are in better agreement with experiment than are the HULLAC results. However, in all cases the $1\sigma$ standard deviation for the ratios of the theoretical-to-experimental resonance strengths is $\gtrsim 30\%$ which is significantly larger than the estimated relative experimental uncertainty of $\lesssim 10\%$. This suggests that similar errors exist in the calculated level populations and line emission spectrum of the recombined ion. We confirm that theoretical methods based on inverse-photoionization calculations (e.g., undamped R-matrix methods) will severely overestimate the strength of the DR process unless they include the effects of radiation damping. We also find that the coupling between the DR and radiative recombination (RR) channels is small.

Below 2 eV the theoretical resonance energies can be up to $\approx 30\%$ larger than experiment. This is larger than the estimated uncertainty in the experimental energy scale ($\lesssim 0.5\%$ below $\approx 25$ eV and $\lesssim 0.2\%$ for higher energies) and is attributed to uncertainties in the calculations. These discrepancies make DR of Fe XX an excellent case for testing atomic structure calculations of ions with partially filled shells. Above 2 eV, agreement between theory and experiment improves dramatically with the AUTOSTRUCTURE and MCDF results falling within 2% of experiment, the R-matrix results within 3%, and HULLAC within 5%. Agreement for all four calculations improves as the resonance energy increases.

We have used our experimental and theoretical results to produce Maxwellian-averaged rate coefficients for $\Delta N = 0$ DR of Fe XX. For $k_B T_e \gtrsim 1$ eV, which includes the predicted formation temperatures for Fe XX in an optically thin, low-density photoionized plasma with cosmic abundances, the experimental and theoretical results agree to better than $\approx 15\%$. This is within the total estimated experimental uncertainty limits of $\lesssim 20\%$. Agreement below $\approx 1$ eV is difficult to quantify due to current theoretical and experimental limitations. Agreement with previously published LS-coupling rate coefficients is poor, particularly for $k_B T_e \lesssim 80$ eV. This is attributed to errors in the resonance energies of these calculations as well as the omission of DR via $2p_{1/2} \rightarrow 2p_{3/2}$ core excitations. We have also used our R-matrix results, topped off using AUTOSTRUCTURE for RR into $J \geq 25$ levels, to calculate the rate coefficient for RR of Fe XX. Our RR results are in good agreement with previously published calculations. We find that for temperatures as low as $k_B T_e \approx 10^{-3}$ eV, DR still dominates over RR for this system.

Subject headings: atomic data – atomic processes
1. Introduction

Low temperature dielectronic recombination (DR) is the dominant recombination mechanism for most ions in photoionized cosmic plasmas (Ferland et al. 1998). Reliably modeling and interpreting spectra from these plasmas requires accurate low temperature DR rate coefficients. Of particular importance are the DR rate coefficients for the iron L-shell ions (Fe XVII-Fe XXIV). These ions are predicted to play an important role in determining the thermal structure and line emission of X-ray photoionized plasmas (Hess, Kahn, & Paerels 1997; Savin et al. 1999, 2000) which are predicted to form in the media surrounding accretion powered sources such as X-ray binaries (XRBs), active galactic nuclei (AGN), and cataclysmic variables (Kallman & Bautista 2001).

The need for reliable DR data for iron L-shell ions has become particularly urgent with the recent launches of Chandra and XMM-Newton. These satellites are now providing high-resolution X-ray spectra from a wide range of X-ray photoionized sources. Examples of the high quality of the data that these satellites are collecting are given by the recent Chandra observations of the XRB Cyg X-3 (Paerels et al. 2000) and the AGN NGC 3783 (Kaspi et al. 2000) and the XMM-Newton observations of the AGN NGC 1068 (Kinkhabwala et al. 2001) and the low-mass XRB EXO 0748-67 (Cottam et al. 2001). Interpreting the spectra from these and other photoionized sources will require reliable DR rate coefficients.

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. The electron excitation can be labeled \( Nl_j \rightarrow N' l'_{j'} \) where \( N \) is the principal quantum number of the core electron, \( l \) its orbital angular momentum, and \( j \) its total angular momentum. This intermediate state, formed by the 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. Conservation of energy requires that for DR to go forward \( E_k = \Delta E - E_b \). Here \( E_k \) is the kinetic energy of the incident electron, \( \Delta E \) the excitation energy of the initially bound electron, and \( E_b \) the binding energy released when the incident electron is captured onto the excited ion. Because \( \Delta E \) and \( E_b \) are quantized, DR is a resonant process. DR via \( N' = 2 \rightarrow N = 2 \) core excitations (i.e., \( \Delta N \equiv N' - N = 0 \) DR) generally dominates the DR process for iron L-shell ions in photoionized plasmas (Savin et al. 1997, 2000).

To address the need for accurate low temperature DR rate coefficients for the iron L-shell ions, we have initiated a program of measurements for DR via \( 2 \rightarrow 2 \) core excitations using the heavy-ion Test Storage Ring (TSR) located at the Max-Planck-Institute for Nuclear Physics in Heidelberg, Germany (Müller & Wolf 1997). To date measurements have been carried out for \( \Delta N = 0 \) DR of Fe XVIII (Savin et al. 1997, 1999), Fe XIX (Savin et al. 1999),
Fe XX, Fe XXI, and Fe XXII. Here we present our results for \( \Delta N = 0 \) DR of Fe XX forming Fe XIX. Preliminary results were presented in Savin et al. (2000). Results for Fe XXI and Fe XXII will be given in future publications.

\( \Delta N = 0 \) DR of nitrogenlike Fe XX can proceed via a number of intermediate resonance states. DR occurs when the autoionizing Fe XIX states, produced in the dielectronic capture process, radiatively stabilize to a bound configuration. Here \( \Delta N = 0 \) captures led to measurable DR resonances for electron-ion collision energies between 0 and \( \approx 105 \) eV and involved the following resonances

\[
\text{Fe}^{19+}(2s^22p^3[^4S_{3/2}]) + e^- \rightarrow \begin{cases} 
\text{Fe}^{18+}(2s^22p[^2D_{3/2}]n^l) & (n = 17, \ldots, \infty) \\
\text{Fe}^{18+}(2s^22p[^2D_{5/2}]n^l) & (n = 15, \ldots, \infty) \\
\text{Fe}^{18+}(2s^22p[^2P_{1/2}]n^l) & (n = 13, \ldots, \infty) \\
\text{Fe}^{18+}(2s^22p[^2P_{3/2}]n^l) & (n = 12, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^4P_{3/2}]n^l) & (n = 8, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^4P_{1/2}]n^l) & (n = 7, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^2D_{3/2}]n^l) & (n = 7, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^2D_{5/2}]n^l) & (n = 7, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^2P_{1/2}]n^l) & (n = 6, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^2P_{3/2}]n^l) & (n = 6, \ldots, \infty) \\
\text{Fe}^{18+}(2s^2p[^2P_{1/2}]n^l) & (n = 6, \ldots, \infty).
\end{cases}
\] (1)

The lowest lying \( \Delta N = 1 \) resonances are predicted to occur at \( E_k \approx 245 \) eV. The excitation energies \( \Delta E \) for all Fe XX levels in the \( n = 2 \) shell are listed, relative to the ground state, in Table 1.

The experimental technique used here is presented in § 2. Our results are given in § 3. Existing and new theoretical calculations are discussed in § 4. A comparison between theory and our experimental results is given in § 5 and conclusions in § 6.

## 2. Experimental Technique

DR measurements are carried out by merging, in one of the straight sections of TSR, a circulating ion beam with an electron beam. After demerging, recombined ions are separated from the stored ions using a dipole magnet and directed onto a detector. The relative electron-ion collision energy can be precisely controlled and the recombination signal measured as a function of this energy. Details of the experimental setup have been given elsewhere (Kilgus et al. 1992; Lampert et al. 1996; Savin et al. 1997, 1999). Here we discuss only those
new details of the setup which were specific to our Fe XX results.

A beam of 280 MeV $^{56}$Fe$^{19+}$ ions was produced and injected into TSR by the usual techniques. Stored ion currents of between $\approx 7 - 22 \mu$A were achieved. The storage lifetime was $\approx 7$ s. After injection, the ions were cooled for $\approx 2$ s before data collection began. This is long compared to the lifetimes of the various Fe XX metastable levels (Cheng, Kim, & Desclaux 1979) and all ions were assumed to be in their ground state for the measurements.

The electron beam was adiabatically expanded from a diameter of $\approx 0.95$ cm at the electron gun cathode to $\approx 3.6$ cm before it was merged with the ions. In the merged-beams region, the electrons were guided with a magnetic field of $\approx 40$ mT and traveled co-linear with the stored ions for a distance of $L \approx 1.5$ m. The effective energy spread associated with the relative motion between the ions and the electrons corresponds to temperatures of $k_B T_\perp \approx 15$ meV perpendicular to the confining magnetic field and $k_B T_\parallel \approx 0.13$ meV parallel to the magnetic field. The electron density varied between $n_e \approx 1 - 3 \times 10^7$ cm$^{-3}$.

Data were collected using three different schemes for chopping the electron beam between the energies for cooling ($E_c$), measurement ($E_m$), and reference ($E_r$). For center-of-mass collision energies $E_{cm} \lesssim 0.048$ eV, the chopping pattern (Mode A) began by jumping to $E_c$ and allowing for a 1.5 ms settling time of the power supplies, followed by a simultaneous cooling of the ions and collecting of data for 30 ms. This was followed by a jump to $E_m$, allowing for a 1.5 ms settling time, and then collecting data for 5 ms. The pattern was completed by jumping to $E_r$, allowing for a 1.5 ms settling time, and then collecting data for 5 ms. For $E_{cm} \gtrsim 0.048$ eV, two different chopping patterns were used. Mode B was similar to Mode A except that when jumping to $E_m$, a settling time of 20 ms was used, and data were then collected for 20 ms. Mode C was similar to Mode B except an $E_c - E_r - E_m$ chopping pattern was used. The chopping pattern was repeated $\approx 300$ times between injections of new ion current. With each step in the chopping pattern, $E_m$ was increased (or decreased) in the lab frame by $\approx 0.5$ eV. The electron energy was stepped by this amount for all three modes.

The reference energy $E_r$ was chosen so that radiative recombination (RR) and DR contributed insignificantly to the recombination counts collected at $E_r$. This count rate was due to essentially only charge transfer (CT) of the ion beam off the rest gas in TSR. Taking electron beam space charge effects into account, the reference energy was $\approx 1600$ eV greater than the cooling energy of $\approx 2740$ eV. This corresponds to an $E_{cm} \approx 183$ eV.

Center-of-mass collision energies were calculated using the velocities of the electrons and the ions in the overlap region. The electron velocity was calculated using the calibrated acceleration voltage and correcting for the effects of space charge in the electron beam.
using the beam energy and diameter and the measured beam current. The ion velocity is determined by the electron velocity at cooling.

For Fe XX, the DR resonance energies measured using Mode C did not precisely match those measured using Mode B. In the lab frame, resonances measured using Mode C occurred at energies $\approx 1.0 - 1.5$ eV lower than those using Mode B. This shift is attributed to $E_r$ preceding $E_m$ for mode C versus $E_c$ preceding $E_m$ in mode B. Capacitances in the electron cooler prevented the acceleration voltage from reaching the desired value in the time allotted. For the data collected here, $E_c$ was essentially always smaller than $E_m$ and $E_r$ was always larger than $E_m$. Hence in mode B, when the beam energy was chopped from $E_c$ up to $E_m$, the cooler capacitances prevented the beam energy from increasing all the way to $E_m$ and the true electron beam energy was slightly less than expected. Conversely, in mode C when the beam energy was chopped from $E_r$ down to $E_m$, these capacitances prevented the beam energy from decreasing all the way to $E_m$ and the true beam energy was slightly higher than expected. $E_{cm}$ was calculated using the expected electron beam energy. Thus the calculated energies in mode B were slightly too high and in mode C slightly too low. To merge the Mode B and Mode C data sets we shifted the Mode C data up in energy, in the lab frame, by $\approx 1.0$ eV at moderate energies and $\approx 1.5$ eV at higher energies. Technical reasons for the occurrence of these voltage errors have been identified and corrected.

The systematic inaccuracies in the absolute $E_{cm}$ scale derived from the voltage calibrations were $\lesssim 2\%$. To increase the accuracy of the $E_{cm}$ scale, a final normalization of the $E_{cm}$ scale was performed using calculated energies for the DR resonances,

$$E_{nl} = \Delta E - \left(\frac{z}{n - \mu_l}\right)^2 \mathcal{R}. \quad (2)$$

Here $E_{nl}$ is the resonance energy for DR into a given $nl$ level, $z$ the charge of the ion before DR, $\mu_l$ the quantum defect for the recombined ion, and $\mathcal{R}$ the Rydberg energy. Values for $\Delta E$ were taken from spectroscopic measurements (Sugar & Corliss 1985) as listed in Table 1. The quantum defects account for energy shifts of those $l$ levels which have a significant overlap with the ion core and cannot be described using the uncorrected Rydberg formula. As $l$ increases, the overlap with the ion core decreases and $\mu_l$ goes to zero.

For the normalization of the $E_{cm}$ scale we used DR resonances with $n \geq 7$ which were essentially unblended with other resonances. We considered only the high-$l$ contributions occurring at the highest energy of a given $n$ manifold, for which $\mu_l$ is essentially zero. The resulting calculated resonance energies were $\approx 1.046$ times the experimental energy scale for $E_{cm} \approx 0.17$ eV. This factor decreased nonlinearly with increasing energy to $\approx 1.016$ at $\approx 10$ eV and then slowly decreased to $\approx 1.003$ with increasing energy. We multiplied the experimental energy scale by this energy-dependent normalization factor to produce the
final energy scale for the results presented here. After corrections, we estimate that above \( \approx 25 \text{ eV} \), the uncertainty in the corrected energy scale is \( \lesssim 0.2\% \). Below \( \approx 25 \text{ eV} \), it is estimated to be \( \lesssim 0.5\% \).

The electron and ion beams were merged and then, after passing through the interaction region, they were separated using toroidal magnets. The motional electric fields in the downstream toroidal magnet field-ionized electrons which had dielectronically recombined into Rydberg levels \( n \gtrsim n_{\text{cut}1} = 146 \). Further downstream, two correction dipole magnets field-ionized electrons in levels \( n \gtrsim n_{\text{cut}2} = 120 \). Finally, the recombined ions passed through a dipole which separated them from the primary ion beam and directed them onto a detector. Electrons in \( n \gtrsim n_{\text{cut}3} = 64 \) were field ionized by this magnet. The flight time of the ions from the center of the interaction region to the final dipole magnet was \( \approx 166 \text{ ns} \). During this time some of the captured electrons radiatively decayed below the various values of \( n_{\text{cut}} \). DR occurs primarily into \( l \lesssim 8 \) levels. Using the hydrogenic formula for radiative lifetimes of Marxer & Spruch (1991), we estimate that for DR into \( n \lesssim n_{\text{max}} = 120 \), the captured electrons radiatively decayed below the various values of \( n_{\text{cut}} \) before reaching the final dipole and were therefore detected by our experimental arrangement.

The measured recombination signal rate was calculated by taking the rate at the measurement energy \( R(E_{cm}) \) and subtracting from it the corresponding rate at the reference energy \( R(E_{ref}) \). This eliminates the effects of slow pressure variations during the scanning of the measurement energy but not the effects of any fast pressure variations associated with the chopping of the electron beam energy, leaving a small residual CT background. Following Schippers et al. (2001), the measured rate coefficient \( \alpha(E_{cm}) \) is given by

\[
\alpha_L(E_{cm}) = \frac{[R(E_{cm}) - R(E_{ref})] \gamma^2}{n_e N_i (L/C) \eta} + \alpha(E_{ref}) \frac{n_e(E_{ref})}{n_e(E_{cm})}.
\]

Here \( N_i \) is the number of ions stored in the ring, \( C = 55.4 \text{ m} \) the circumference of the ring, \( \eta \) the detection efficiency of the recombined ions (which is essentially 1), \( \gamma^2 = [1 - (v/c)^2]^{-1} \approx 1.01 \), and \( c \) the speed of light. The measured rate coefficient represents the DR and RR cross sections multiplied by the relative electron-ion velocity and then convolved with the experimental energy spread. The data sit on top of the residual CT background. The experimental energy spread is best described by an anisotropic Maxwellian distribution in the comoving frame of the electron beam. The second term in Equation 3 is a small correction to re-add the RR signal at the reference which is subtracted out in the expression \( [R(E_{cm}) - R(E_{ref})] \). Here we used the theoretical RR rate coefficient at \( E_{cm} = 183 \text{ eV} \) where contributions due to DR are insignificant. The RR rate coefficient at this energy, calculated using a modified semi-classical formula for the RR cross section (Schippers et al. 1998), is \( \approx 4.3 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1} \). Using \( \alpha_L(E_{cm}) \), the effects of the merging and demerging of the
electron and ion beams are accounted for, following the procedure described in Lampert et al. (1996), to produce a final measured recombination rate coefficient $\alpha(E_{cm})$ from which the DR results are extracted.

The DR resonances produce peaks in $\alpha(E_{cm})$. Resonance strengths are extracted after subtracting out the smooth background due to RR and CT. Although RR dominates the smooth background at low energies, we have been unable to extract reliable RR rate coefficients due to the remaining CT contributions to the measured signal rate.

Experimental uncertainties have been discussed in detail elsewhere (Kilgus et al. 1992; Lampert et al. 1996). The total systematic uncertainty in our absolute DR measurements is estimated to be $\lesssim 20\%$. The major sources of uncertainties include the electron beam density determination, the ion current measurement, corrections for the merging and de-merging of the two beams, the efficiency of the recombined ion detector, resonance strength fitting uncertainties, and uncertainties in the shape of the interpolated smooth background (particularly in regions where the DR resonances were so numerous that the background was not directly observable). Another source of uncertainty is that we assume each DR feature can be fit using a single resonance peak when in fact each feature is often composed of many unresolved resonance peaks. Relative uncertainties for comparing our DR results at different energies are estimated to be $\lesssim 10\%$. Uncertainties are quoted at a confidence level believed to be equivalent to a 90\% counting statistics confidence level.

3. Experimental Results

Our measured spectrum of Fe XX to Fe XIX $\Delta N = 0$ DR resonances is shown in Figure 1(a). The data represent the sum of the RR and DR cross sections times the relative electron-ion velocity convolved with the energy spread of the experiment, i.e., a rate coefficient. The data are presented as a function of $E_{cm}$. For energies below 7.5 eV, we use the predicted asymmetric line shape for the DR resonances (Kilgus et al. 1992) and fit the data to extract DR resonance strengths and energies. Above 7.5 eV, the asymmetry is insignificant and we fit the data using Gaussian line shapes. Extracted resonance strengths $S_d$ and energies $E_d$ for a given DR resonance or blend of resonances $d$ are listed in Table 2. The energies have been corrected as described in § 2.

The lowest-energy resolved resonance is the $2s^22p^3(2D_{3/2})17l$ blend at $E_{cm} \approx 0.081$ eV. Our fit to this blend begins to deviate significantly from the measured data for $E_{cm} \lesssim 0.05$ eV (see Figure 2). We attribute this deviation to unresolved broad and narrow DR resonances lying below 0.05 eV.
Due to the energy spread of the electron beam, resonances below \( E_{\text{cm}} \approx k_B T_e \approx 0.015 \text{ eV} \) cannot be resolved from the near 0 eV RR signal. However, we can infer the presence of such resonances. The measured recombination rate coefficient at \( E_{\text{cm}} \lesssim 10^{-4} \text{ eV} \) is a factor of \( \approx 90 \) times larger than the RR rate coefficient predicted using semiclassical RR theory with quantum mechanical corrections (Schippers et al. 1998). This enhancement factor is much larger than that found for Fe XVIII for which the near 0 eV recombination rate coefficient was a factor of \( \approx 2.9 \) times larger than the theoretical RR rate coefficient. Fe XVIII is predicted to have no DR resonances near 0 eV. A similar enhancement (factor of \( \approx 2.2 \)) was found for RR of bare Cl XVIII (Hoffknecht et al. 2001). For Fe XIX, the enhancement was a factor of \( \approx 10 \). Fe XIX and Fe XX are both predicted to have near 0 eV DR resonances and the inferred enhancement factors of greater than 2.9 are attributed to these unresolved near 0 eV resonances.

We note that a number of issues pertaining to recombination measurements in electron coolers at \( E_{\text{cm}} \lesssim k_B T_e \) remain to be resolved (Hoffknecht et al. 1998; Schippers et al. 1998; Gwinner et al. 2000; Hoffknecht et al. 2001), but it is highly unlikely that their resolution will lead to a near 0 eV recombination rate coefficient that increases by a factor of \( \approx 30 \) for a change in ionic charge from 17 to 19. Thus we infer that there are unresolved DR resonances lying at energies below 0.015 eV.

Our calculations suggest that these unresolved resonances are due to a combination of the \( 2s^22p^3(2D_{5/2})15l \) and \( 2s2p^4(4P_{3/2})7d \) configurations. Calculations indicate these \( 15l \) resonances have natural line widths significantly smaller than the energy spread of the experiment. Here we treat them as delta functions for fitting purposes. To determine the energies of these \( 15l \) resonances, we use the calculated quantum defect for an \( nf \) electron in Fe XIX from Theodosiou et al. (1986). The \( f \) level is the highest angular momentum they considered. We extrapolate this quantum defect to higher angular momentum using the predicted \( l^{-1} \) behavior (Babb et al. 1992). The resulting resonance energies are listed in Table 2. We estimate that for this complex, the \( 15i \) level is the lowest lying DR resonance. The highest resonance energy (for the \( 15l \) level) is estimated to be at \( \approx 0.005 \text{ eV} \).

The energy of the near 0 eV \( 2s2p^4(4P_{3/2})7d \) resonance is difficult to predict reliably because of the large interaction of the captured electron with the core. Calculations indicate the resonance has a width of \( \approx 10 \text{ meV} \) which is comparable to the energy spread of the experiment. To fit for this feature we must take the natural line profile of the DR resonance and its \( E_{\text{cm}}^{-1} \) dependence into account. Mitnik et al. (1999) have addressed theoretically the issue of near 0 eV DR resonances. Starting from Equation 12 of their paper, we can write...
the near 0 eV DR line profile as

$$
\sigma_{DR}(E_{cm}) = \frac{S_d E_d}{E_{cm}} \left[ \frac{\Gamma_d/2\pi}{(E_{cm} - E_d)^2 + (\Gamma_d/2)^2} \right]
$$

where $\Gamma_d$ is the natural line width of the resonance.

Recent measurements of recombination of bare Cl XVIII found an enhanced recombination rate coefficient for $E_{cm} \lesssim 0.008$ eV (Hoffknecht et al. 2001). We expect a similar situation for Fe XX. Because the unresolved 15$l$ DR resonances all occur for $E_{cm} \lesssim 0.005$ eV, we attribute the DR signal between 0.008 and 0.05 eV to the unresolved 7$d$ resonance. We have fit this portion of the recombination spectrum essentially by eye, varying the resonance width, strength, and energy. Our best fit was for an inferred resonance width of 10 meV. The inferred resonance energy and strength of this 7$d$ resonances are listed in Table 2.

Based on our Fe XVIII results (Savin et al. 1997, 1999), we expect to see an enhancement of $\approx 2.9$ as $E_{cm}$ approaches 0 eV. Taking only the near 0 eV 7$d$ resonance into account yields an enhancement factor of $\approx 6.7$. We infer the resonance strength of the near 0 eV 15$l$ resonances by varying their amplitudes to produce a model recombination spectrum which yields an enhancement factor of $\approx 2.9$.

We have linked the resonance strengths of the near 0 eV 15$l$ levels taking into account the behavior of the DR cross section. Following the logic in § II of Müller et al. (1987), when the radiative stabilization rate $A_r$ is much greater than the autoionization rate $A_a$ of the intermediate doubly-excited state in the DR process, then the DR resonance strength is proportional to $A_a$. For the $2s^22p^3(^2D_5/2)15l$, the excited core electron cannot decay via an electric dipole transition. Stabilization of the intermediate autoionizing state is due to a radiative decay by the Rydberg electron. Using the hydrogenic formula of Marxer & Spruch (1991) for the radiative lifetime of the 15$l$ electron and our calculated MCDF autoionization rates, we find that the radiative rates are always significantly larger than the autoionization rates. We have therefore linked the relative resonance strengths for the near 0 eV 15$l$ resonances using the MCDF calculated $A_a$ values. Thus the amplitudes of these resonances are controlled by a single normalization factor. We have varied this factor until our model recombination spectrum yields an enhancement factor of $\approx 2.9$ for $E_{cm} < 10^{-4}$ eV. The inferred resonance strengths for these 15$l$ resonances are listed in Table 2.

The measured and model recombination spectrum below $E_{cm} = 0.1$ eV is shown in Figure 2. For the model spectrum we use our inferred and extracted resonance strengths and energies. We have looked at the difference between the measured and model spectrum between 0.008 and 0.05 eV. The resulting residuals are comparable to the difference between the measured spectrum and the fitted spectrum for those peaks below 1 eV which we were
able to fit using a $\chi^2$ procedure. We note here that the 10 meV width of this resonances is significantly larger than our fitted resonance energy of 3 meV. Thus we infer that the DR cross section is non-zero in value for $E_{cm} = 0$ eV and that the resulting Maxwellian DR rate coefficient will increase as the plasma temperature decreases.

We have used the extracted DR resonance strengths and energies listed in Table 2 to produce a rate coefficient for $\Delta N = 0$ DR of Fe XX forming Fe XIX in a plasma with a Maxwellian electron energy distribution at a temperature $T_e$. We treated all resonances listed, except for the near 0 eV 7d resonance, as delta functions. Using these resonances and the measured unresolved resonances near the series limit, we have produced a rate coefficient following the procedure described in Savin (1999). To this we have added the rate coefficient due to the 7d resonance. This rate coefficient is calculated using Equation 4 multiplied by the relative electron-ion velocity and integrating this over a Maxwellian distribution. The resulting $\Delta N = 0$ rate coefficient is shown in Figure 3(a). The inferred contribution due to the near 0 eV 15l and 7d resonances is $\approx 81\%$ at $k_B T_e = 0.1$ eV, $\approx 18\%$ at 1 eV, $\approx 4\%$ at 10 eV, and $\approx 1\%$ at 100 eV. We estimate the uncertainty in our experimentally-derived rate coefficient to be $\lesssim 20\%$ for $k_B T_e \gtrsim 1$ eV. At lower temperatures, the uncertainty of the strengths for the near 0 eV resonances causes a larger uncertainty which is is difficult to quantify.

We have fitted our experimentally-derived $\Delta N = 0$ DR rate coefficient using

$$\alpha_{DR}(T_e) = T_e^{-3/2} \sum_i c_i e^{-E_i/k_B T_e}$$

where $T_e$ is given in units of K. Table 3 lists the best-fit values for the fit parameters. The fit is good to better than 1.5% for $0.001 \leq k_B T_e \leq 10000$ eV. Although we infer above that the DR rate coefficient is non-zero at $k_B T_e = 0$ eV, our fitted DR rate coefficient eventually goes to 0 for $k_B T_e < 0.001$ eV. However, we expect this to have no significant effect on plasma modeling as it is extremely unlikely that Fe XX will ever form at temperatures below 0.001 eV (Kallman & Bautista 2001).

4. Theory

Existing theoretical rate coefficients for DR of Fe XX have been calculated in LS-coupling. Shull & van Steenberg (1982) present the fitted results of Jacobs et al. (1977). Arnaud & Raymond (1992) present the unpublished results of Roszman. Details of the theoretical techniques used for the calculations can be found in Jacobs et al. (1977) and Roszman (1987) and references therein.
There have been major theoretical advances in the study of DR since the works of Jacobs et al. and Roszman. We have carried out new calculations using AUTOSTRUCTURE, HULLAC, MCDF, and R-matrix methods, four different state-of-the-art theoretical techniques. Below we briefly describe these techniques and the results.

4.1. AUTOSTRUCTURE

DR cross section calculations were carried out in the independent-processes, isolated-resonance approximation using the code AUTOSTRUCTURE (Badnell 1986). This technique treats both the electron-electron (repulsive Coulomb) operator

\[ V = \sum_{\alpha\beta} \frac{1}{|\mathbf{r}_\alpha - \mathbf{r}_\beta|} \]

and the electron-photon (electric dipole) operator

\[ \vec{D} = \sqrt{2\omega/3\pi c^3} \sum_{\alpha} \mathbf{r}_\alpha \] to first order. The subscripts \( \alpha \) and \( \beta \) are electron labels and \( \omega \) is the emitted photon energy.

All continuum wavefunctions \( 2l^5\ell' \), and all resonance or bound wavefunctions \( 2l^5nl' \), were constructed within the distorted-wave approximation. The resulting wavefunctions were used to calculate all autoionization rates

\[ \Gamma_{d_i} = 2\pi \left| \langle 2l^5n_d|V|2l^5\epsilon_i'\ell_i' \rangle \right|^2 \]

and radiative rates

\[ \Gamma_{r_{df}} = 2\pi \left| \langle 2l^5n_d|\vec{D}|2l^5\epsilon_f\ell_f \rangle \right|^2 \].

Here the subscript \( i \) denotes the continuum states (\( i = 1 \) is the initial free electron plus the initial ionic system), \( d \) denotes the resonance states, and \( f \) denotes the final recombined states. Next, these rates were all used in the analytic expression for the (unconvoluted) DR cross section

\[ \sigma_{DR}(E) = \sum_d \sigma_{DR}^d(E) = \sum_d \frac{2\pi^2}{k^2} \frac{(2J_{d} + 1)}{2(2J_{core} + 1)} \frac{\Gamma_{d_i}}{\Gamma_{d_f}} \left( \frac{\sum_{f'} \Gamma_{r_{df'}}/2\pi}{(E - E_d)^2 + \left( \frac{\Sigma_i \Gamma_{d_i} + \Sigma_{f'} \Gamma_{r_{df'}}}{2} \right)^2} \right) \]

which is a function of electron kinetic energy \( E = \frac{1}{2}k^2 \) relative to the initial state (e.g., \( i = 1 \)). \( J_{d_f} \) is the total angular momentum of the resonance state, \( J_{core} = 3/2 \) the angular momentum of the \( 1s^22s^22p^3(4S_{3/2}) \) initial core ionic state, and \( E_d \) the energy of the resonance state. The continuum wavefunctions are energy normalized such that

\[ \langle \epsilon | \epsilon' \rangle = \delta(\epsilon - \epsilon') \delta_{ll'} \].

The sum over \( f' \) in the numerator only includes radiative transitions to bound states. Radiative decay to states that subsequently autoionize make rather small contributions to the DR process and are only included in the sum over \( f \) in the denominator.

For the initial atomic structure, the \( 1s, 2s, \) and \( 2p \) orbitals making up all possible \( 2l^5(2S+1L_f) \) ionic states, as well as the \( 2l^6 \) recombined states, were determined from a Hartree-Fock (Froese-Fischer 1991) calculation for the \( 1s^22s^22p^3(4S) \) ground state of Fe XX. The 7 and 8 electron atomic structures were obtained by diagonalizing the appropriate Breit-Pauli Hamiltonian. Calculated ionic Fe XX energies are listed in Table 1. Prior to the final DR
cross section calculations, these ionic thresholds were shifted to the known spectroscopic values (Sugar & Corliss 1985) by \( \lesssim 2.5 \) eV. The \( \epsilon_l n'_l \) and \( n f l'_f \) orbitals were subsequently determined from single-configuration continuum and bound distorted wave calculations, respectively. We included explicitly all orbital angular momentum and principal quantum numbers in the range \( 0 \leq l' \leq 17 \) and \( 6 \leq n \leq 120 \). Configuration mixing was minimal in these calculations. Only the \( 2l^6 \) bound states were coupled to each other. All other \( 2l^5 n l' \) resonances, for all \( n > 6 \) and \( l' \), were treated as non-interacting resonances.

The DR cross section is the sum of Lorentzian profiles. This analytic cross section can also be energy integrated to give resonance strengths or convoluted with the experimental energy distribution for comparison with the measured results. DR rate coefficients can be obtained by convolving the DR cross section with a Maxwellian electron distribution.

### 4.2. HULLAC

DR resonance strengths are calculated in the independent processes, isolated resonance, and low-density approximations. The DR cross section can then be written as the product of the cross section for dielectronic capture and the branching ratio for subsequent radiative stabilization. In the low-density limit, the branching ratio includes only radiative and autoionization decays. Basic atomic quantities are obtained using the multi-configuration HULLAC (Hebrew University Lawrence Livermore Atomic Code) computer package (Bar-Shalom et al. 2001). The calculations employ a relativistic parametric potential method for the atomic energy levels (Klapisch 1971; Klapisch et al. 1977) while using first order perturbation theory for the radiative decay rates. The autoionization rates are calculated in the distorted wave approximation, implementing a highly efficient factorization-interpolation method (Bar-Shalom et al. 1988; Oreg et al. 1991). Full configuration mixing is included within and between the configuration complexes \( 1s^2 2l^5 n' l' (n' \leq 6) \). For the \( 1s^2 2l^5 n' l' (n' > 6) \) complexes, only mixings within a given \( n' \)-complex are included. Mixing between complexes with different \( n' \) values for \( n' > 6 \) has only a minor effect and is neglected.

All of the dielectronic capture channels from the Fe XX ground level \( 1s^2 2s^2 2p^3 \, 4S_{3/2}^o \) to the Fe XIX doubly excited levels \( 1s^2 2l^5 n' l' \) are included. These include the fine-structure core excitations (i.e., \( 2p_{1/2} - 2p_{3/2} \) core transitions). Explicit calculations are performed for \( 6 \leq n' \leq 25 \), and \( l' \leq 9 \). DR contributions from \( 1s^2 2l^5 n' l' (n' > 25) \) configurations are estimated by applying the \( n'^{-3} \) scaling law to the individual autoionization and radiative transition rates when the \( n' \) electron is involved. Calculated Fe XX energy levels are listed in Table 1. These correspond to the various series limit energies for \( \Delta N = 0 \) DR. Prior to the final DR cross section calculations, the theoretical resonance energies have been adjusted.
by $\lesssim 2.1$ eV so that the series limits match the spectroscopically measured energies (Sugar & Corliss 1985). All possible autoionization processes to $1s^22l^5$ levels following the initial dielectronic capture are accounted for, including those to excited states. All of the radiative decays to non-autoionizing levels are included in the branching ratio. Radiative cascades to autoionizing levels, on the average, can be shown to have little effect on the calculated branching ratios (Behar et al. 1995, 1996). Throughout this work only the electric dipole radiative transitions are computed. The calculated DR cross sections are folded with a Maxwellian distribution of the plasma electrons to obtain the DR rate coefficients.

4.3. Multiconfiguration Dirac-Fock (MCDF)

DR calculations are carried out in the independent process, isolated resonance approximation (Seaton & Storey 1976). In these approximations, the interference between DR and RR is neglected and the effects of interacting resonances are ignored. The DR cross section can then be written as a product of the resonance capture cross section and the stabilizing radiative branching ratio. The required energy levels and Auger and radiative transition rates for the autoionizing states are obtained using the Multiconfiguration Dirac-Fock (MCDF) method (Grant et al. 1980; Chen 1985). These calculations are carried out in the average-level scheme and in intermediate coupling with configuration interaction within the same principal quantum $n$ complex. All possible Coster-Kronig channels and radiative decays to bound states are included. A one-step cascade correction is taken into account when the radiative decay of the core electron leads to an autoionizing state.

We include excitation from the ground state $1s^22s^22p^3\,^4S_{3/2}$ to the $1s^22s^22p^3\,^2P, ^2D$ and $1s^22s^22p^4\,^4P, ^2D, ^2S$, and $^2P$ states. For fine-structure core excitations (i.e., $2p_{1/2} - 2p_{3/2}$ core transitions), explicit calculations are performed for $12 \leq n \leq 35$, and $l \leq 12$ autoionizing states. For $2s - 2p$ core excitations, explicit calculations are carried out for $6 \leq n \leq 35$, and $l \leq 12$ states. Contributions from $l > 12$ have been estimated by extrapolating from the $l = 10 - 12$ results. The contributions contribute $< 1\%$ to the total DR rate coefficient and are neglected in the final calculations. Calculated Fe XX energy levels are listed in Table 1. These correspond to the various series limit energies for $\Delta N = 0$ DR. Prior to the final DR cross section calculations, the theoretical resonance energies have been adjusted by $\lesssim 1.5$ eV so that the series limits match the spectroscopically determined excitation energies (Sugar & Corliss 1985). The DR cross sections for $36 \leq n \leq 120$ states are estimated by using the $n^{-3}$ scaling law for the transition rates. DR cross sections with $6 \leq n \leq 120$ have been folded with the Maxwellian distribution of the plasma electrons to obtain the DR rate coefficients.
4.4. R-Matrix

We have also carried out calculations using the Belfast R-matrix codes for the inner region (Burke & Berrington 1993; Berrington et al. 1995) and a modified version of the STGF code for the outer region (Berrington et al. 1987). These include spin-orbit and other Breit-Pauli corrections (Scott & Taylor 1982), and have been extensively modified to include radiation damping (Robicheaux et al. 1995; Gorczyca et al. 1995, 1996), which is crucial for the present case of Fe XX. One appealing aspect of the R-Matrix technique is that the continua and resonances are coupled together as a structured continuum, unlike the perturbative methods that compute resonance and continuum distorted wave orbitals separately. This is achieved somewhat differently depending on the region of configuration space. Inside the so-called R-matrix “box” the total 8 electron wavefunction of Fe XIX is expanded in a large basis, making no distinction between resonance or continuum states. The surface amplitudes at \( r_a \), compactly represented by the R-matrix, are determined from variational considerations. The radius of the “box” used here, \( r_a = 2.2 \) a.u., was chosen in order to include all \( 2p^3l \) bound states. Outside the R-matrix box, the continua and resonances are initially treated as separate Coulomb functions, but are then coupled by the long-range non-Coulombic potential, giving off-diagonal elements to the open-closed scattering matrix of multi-channel quantum defect theory (MQDT). Thus, the outer region wavefunction is also made up of structured continua, once physical boundary conditions are applied. Note that we find the long-range coupling to significantly affect the calculated DR cross section (Gorczyca et al. 1996).

In order to describe how the subsequent radiation from these structured continua are included in the present treatment, it helps to first show all included direct (RR) and resonant (DR) pathways leading to recombination for the case of Fe XX:

\[
e^- + 2s^22p^3(^4S) \rightarrow 2s^22p^3(^4S_{3/2})n'nl' (2 \leq n' \leq 3) \tag{7}
\]
\[
\rightarrow 2l^5nl \rightarrow 2l^5n'l' (2 \leq n' \leq 3) \tag{8}
\]
\[
\rightarrow 2s^22p^3(^4S_{3/2})n'l' (4 \leq n' \leq 120) \tag{9}
\]
\[
\rightarrow 2s2p^4nl \rightarrow 2s^22p^3nl (6 \leq n \leq 120) \tag{10}
\]
\[
\rightarrow 2s2p^4nl \rightarrow 2s2p^4n'l' \pm 1 (4 \leq n' \lesssim 5) \tag{11}
\]
\[
\rightarrow 2s^22p^3snl \rightarrow 2s^22p^3sn'l' \pm 1 (4 \leq n' \lesssim 16). \tag{12}
\]

In the above pathways, the stabilizing photon emitted has been omitted. In Equation 10, the \( 2s2p^4nl \rightarrow 2s^22p^3nl \) radiative transition may leave the core in either its ground state or an excited state. In Equations 11 and 12, the \( \lesssim \) symbols indicate that the exact maximum value of \( n' \) depends on the specific configuration of the core electrons. This value of \( n' \) can be determined from Equation 1 for the different core configurations. The notation \( 2p^3s \) indicates...
that the \(2p^3\) electrons are in an excited configuration.

The direct/resonant processes in Equations 7 and 8, end up in recombined states that reside completely in the R-matrix box. Recombination into these states is treated by using a non-local, energy-dependent, imaginary optical potential in the inner-region Hamiltonian, leading to a complex R-matrix, and therefore a non-unitary S-matrix. Thus, interference between DR and RR is naturally included here. For the direct recombination shown in Equation 9, we add a term \(-i\Gamma_{RR}/2\) to the diagonal open-open elements of the scattering matrix, where \(\Gamma_{RR}\) is computed in the hydrogenic approximation as

\[
\Gamma_{RR} = 2\pi \sum_{n'=4}^{\infty} \sum_{l,l'} |\langle el|D|n'l'\rangle|^2
\]

where \(el\) denotes a continuum orbital.

The RR processes in Equations 7 and 9 are also used to compute a pure RR cross section, but it is important to omit all excited states \(2l^5\) and scatter from the \(2s^22p^3(4S_{3/2})\) target alone, thereby eliminating all DR resonances. Here we used partial waves \(J^{\pi}\) from \(J_{max} = 10\) to \(J_{max} = 25\), for both even and odd parities \(\pi\). In order to get reasonable agreement with the RR results of Arnaud & Raymond (1992), we found it necessary to use a box size big enough to enclose the \(2l^53l'\) states in order that RR to these states was not treated hydrogenically. For these lowest-lying states, the hydrogenic approximation is less valid. Subsequent runs using a box large enough for the \(n = 4\) states, and treating \(n = 5\) and higher hydrogenically changed the calculated RR cross section by less than 2\% (see also the similar discussion by Arnaud & Raymond 1992).

To treat the core radiative decay in Equation 10, where the valence electron acts as a spectator, we modify the effective quantum number \(\nu\) in the closed-channel MQDT expression by adding a term \(-i\Gamma_{core}/2\) to the core energy \(E_{core}\) used in determining \(\nu\). Here \(\nu\) is a continuous variable, calculated using \(E_{cm} = E_{core} - Z^2/2\nu^2\), and \(\Gamma_{core}\) is given by

\[
\Gamma_{core} = 2\pi|\langle 2s2p^4|D|2s^22p^3\rangle|^2,
\]

where \(Z = 19\). We treat the valence decay in Equations 11 and 12 hydrogenically, and add a term \(-i\Gamma_{valence}/2\) to the diagonal closed-closed part of the unphysical scattering matrix, where

\[
\Gamma_{valence} = 2\pi \sum_{n'=4}^{16} \sum_{l' = \pm 1} |\langle nl|D|n'(l \pm 1)\rangle|^2.
\]

Note that there is no interference considered between the RR pathway in Equation 9 and the DR pathways in Equations 10, 11, and 12, but this is expected to be less important than
the interference occurring between Equations 7 and 8 since the RR rate is strongest to the
lowest lying states, and only when the RR and DR rates to the same final recombined state
are comparable will any significant interference occur.

For FVII, Ar XVI, and Fe XXV, the present type of R-matrix calculation has been shown
to give results nearly identical to those from the perturbative code AUTOSTRUCTURE
(Gorczyca et al. 1996; Gorczyca & Badnell 1997; Mitnik et al. 1999). However, in certain
highly-sensitive cases, differences between the two codes can be seen. For DR of Li II
(Saghiri et al. 1999), AUTOSTRUCTURE results were not in as good agreement with the
measurements as were the R-matrix results (Price 1997). In Sc IV, AUTOSTRUCTURE
calculations needed to be extended to include interference effects between RR and DR before
agreement was found with R-matrix results (Gorczyca et al. 1997). One aim of the present
work is to search for possible interference effects in Fe XX where they would most likely
occur (i.e., to short-range final recombined states). However, for highly ionized systems,
such as that studied here, the effects of interference between the RR and DR channels
are unlikely to influence the computed Maxwellian rate coefficient (Pindzola, Badnell, &
Griffin 1992). Indeed by comparing our AUTOSTRUCTURE calculations (which here do
not include interference effects) with our R-matrix results, we find in the present case that
these effects are negligible on the Maxwellian rate coefficient.

R-matrix results are expected to give rise to slightly better autoionization and/or radia-
tive widths, compared to perturbative approaches. This is due to the more flexible R-matrix
basis used to describe the wavefunction of each structured continuum (i.e., continuum with
embedded resonances). The R-matrix atomic structure calculations start with the same 1s,
2s, and 2p orbitals and configurations as described in § 4.1. Hence the calculated level ener-
gies are the same as for our AUTOSTRUCTURE results and prior to the final DR cross
sections calculations, these energies were shifted to the spectroscopically known values (Sugar
& Corliss 1985). We also calculated the 3s, 3p, and 3d orbitals optimized on the 2s^22p^23l
configuration-average energies. These levels were included so that the 2l^53l'' final recombined
states were contained in the R-matrix box (see discussion above). For the resonance and
continuum states all total spin and orbital angular momenta S' = 0 − 2, L' = 0 − 27 (even
and odd parities) were used in LS-coupling, and LS-JK recoupled to include all J' = 0 − 25
(even and odd parities). A basis of 20 R-matrix orbitals was used to describe each continuum
el' or bound nl' orbital.

Using the radiation-damped R-matrix approach, the photorecombination cross section
is computed as the flux lost through the electron-ion scattering process. Due to the inclusion
of a radiative optical potential in the R-matrix Hamiltonian (Robicheaux et al. 1995), the
scattering matrix S(E) is no longer unitary, and its non-orthogonality can be related to the
photorecombination cross section as

\[ \sigma_{PR}(E) = \sum_d \frac{\pi}{k^2} \frac{(2J_d' + 1)}{2(2J_{\text{core}} + 1)} \sum_{\alpha} \left\{ 1 - \sum_{\beta} S_{\alpha\beta}^*(E)S_{\alpha\beta}(E) \right\}, \tag{16} \]

where \(\alpha\) is summed over all channels coupled to the initial ionic target state \(2s^22p^3(^4S_{3/2})\) and \(\beta\) is summed over all open, or continuum, channels. The closed, or resonance, channels have been incorporated into this scattering information via MQDT (Seaton 1983; Aymar, Greene, & Luc-Koenig 1996). In the absence of all couplings except for the resonance-continuum terms, Equation 16 reduces to the DR term in Equation 6 plus the direct RR term and the RR/DR interference term for those final recombined states that reside in the box. If all resonance states, contained in the closed-channels, are omitted from the R-matrix expansion, Equation 16 yields just the RR cross section. These RR results are used for the non-resonant background to produce RR+DR results for our AUTOSTRUCTURE, HULLAC, and MCDF results.

In order to resolve the many very narrow resonances, whose energy positions are not known analytically, the scattering matrix \(S(E)\) in Equation 16 needs to be evaluated at an enormous number of energy points. This is to be contrasted with the AUTOSTRUCTURE, HULLAC, and MCDF calculations which analytically determine the resonance energies from a distorted wave bound state eigenvalue solution, that neglects the accessible continua. For the present R-matrix results, we used 800,000 points to cover the energy range \(0 \leq E \leq 120\) eV; this gave an energy-mesh spacing of \(1.5 \times 10^{-4}\) eV, which is comparable to the \(2s2p^4nl \rightarrow 2s^22p^3nl\) core radiative decay width. MQDT methods have been used to minimize the computational work. Even with this more efficient method, however, about two days of CPU time was required on a dual pentium pro Linux workstation, compared to the AUTOSTRUCTURE time on the same machine of about 40 minutes.

Our R-matrix results include the effects of radiation damping. Despite many of the radiative stabilizing decays here being \(\Delta N = 0\) transitions, using AUTOSTRUCTURE we find radiation damping to be extremely important for Fe XX. Near the Rydberg limits, comparing the AUTOSTRUCTURE results with and without the inclusion of the \(\sum_f \Gamma_{\alpha\beta}^r\) term in the denominator of Equation 6, we find that there is a damping reduction by more than an order of magnitude in the convoluted cross section. Just as importantly, some of the lower-\(n\) resonances are damped by factors of 2 in the convoluted cross section. Hence, theoretical methods based on inverse-photoionization calculations will, without the inclusion of radiation damping, severely overestimate the true cross section, provided that these narrow, undamped resonances are fully resolved in the first place.
4.5. Results

We have multiplied the AUTOSTRUCTURE, HULLAC, and MCDF $\Delta N = 0$ DR cross sections with the relative electron-ion velocity and convolved the results with the TSR energy spread to produce a rate coefficient for direct comparison with our experimental results. We have done the same for the R-matrix RR cross section data and added the results to the AUTOSTRUCTURE, HULLAC, and MCDF DR data. The resulting convolved RR+DR data are shown, respectively, in Figures 1(b), 1(c), and 1(d). The R-matrix results yield a unified RR+DR cross section which we multiplied by the relative electron-ion velocity and convolved with the experimental energy spread. These results are shown in Figure 1(e).

Figure 3(b) shows the AUTOSTRUCTURE, HULLAC, and MCDF $\Delta N = 0$ DR results (for $n_{\text{max}} = 120$) convolved with a Maxwell-Boltzmann electron energy distribution. We have fitted these DR rate coefficients using Equation 5. Table 3 lists the best-fit values for the fit parameters. For $0.001 \leq k_B T_e \leq 10000$ eV, the fit is good to better than 1.5% for the AUTOSTRUCTURE results and 0.8% for the MCDF results. The fit to the HULLAC results is good to better than 0.3% for $0.01 \leq k_B T_e \leq 10000$ eV. Below 0.01 eV, the fit goes to zero faster than the calculated HULLAC rate coefficient.

Because interference between the RR and DR channels appears to be unimportant, we can also produce an R-matrix DR-only rate coefficient ($n_{\text{max}} = 120$) by subtracting the RR-only R-matrix results ($n_{\text{max}} = 120$) from the RR+DR results ($n_{\text{max}} = 120$). In figure 3(b) we show our DR-only ($n_{\text{max}} = 120$) and RR-only ($n_{\text{max}} = \infty$) results. Table 3 lists the best-fit values for the DR fit parameters. For $0.001 \leq k_B T_e \leq 10000$ eV, the fit is good to better than 1.0% for the R-matrix results. Including DR contributions from $n = 120$ to $\infty$ is predicted by us to have an insignificant effect below $k_B T_e = 10$ eV, and to increase our experimentally-derived DR rate coefficient by 1% at 27 eV, by 3% at 65 eV, by 5% at 268 eV, and by 5.6% at 10,000 eV.

Our RR rate coefficient ($n_{\text{max}} = \infty$) is listed in Table 4. In order to converge at energies $\lesssim 1$ eV, we found it necessary to top-up our R-maxtrix RR results with hydrogenic calculations of RR into $J \geq 26$ using AUTOSTRUCTURE.

5. Discussion

Table 1 gives the experimental and theoretical energies for all Fe XX $n = 2$ levels. The spectroscopically derived energies of Sugar & Corliss (1985) are listed first. Also given are the unshifted energies calculated using the AUTOSTRUCTURE, HULLAC, and MCDF techniques as well as from calculations by Bhatia et al. (1989), Donnelly et al. (1999), and
Zhang & Pradhan (2000). Our MCDF energies and the results of Zhang & Pradhan agree to within \( \approx 2\% \) with the experimental values. Our AUTOSTRUCTURE, HULLAC, and R-matrix results and those of Bhatia et al. lie within \( \approx 3\% \) of experiment. The energies of Donnelly et al. lie within \( \approx 4\% \) of the experimental values.

AUTOSTRUCTURE, HULLAC, and MCDF calculations use a perturbative technique and yield DR resonance strengths and energies. The R-matrix calculations use a non-perturbative method and yield unified RR+DR recombination results. Comparisons of individual resonance strengths and energies between experiment and theory are most straightforward for perturbative calculations. For these results the energy-integrated resonance strength

\[
S_d = \int_{E_d-\Delta E/2}^{E_d+\Delta E/2} \sigma_{DR}^d(E) dE
\]

(17)
can be calculated in analytic form, thereby giving the contribution from each isolated resonance \( d \). We compare our experimental results with the non-perturbative R-matrix results to the extent that is straightforwardly possible.

DR resonances are identified in Table 2 by their dominant component. AUTOSTRUCTURE, HULLAC, and MCDF results have been used as a guide in the resonance assignment. In general, unambiguous identification is possible. One clear exception is for the \( 2s2p^4(4P_{3/2})7d_{3/2} \ (J = 3) \) and \( 2s2p^4(4P_{3/2})7d_{5/2} \ (J = 3) \) resonances. AUTOSTRUCTURE predicts these resonances to lie, respectively, at \( \approx 0.04 \) and \( \approx 0.3 \) eV. MCDF predicts them at \( \approx 0.3 \) and \( \approx 0.04 \) eV. The ambiguity in resonance assignment is most likely due to strong mixing between these two states. HULLAC predicts the \( 7d_{3/2} \) resonance to occur at \( \approx 0.3 \) eV and that the \( 7d_{5/2} \) level lies below the Fe XIX continuum. Our fit to the unresolved near 0 eV recombination signal suggests this latter resonance is broad and straddles the ionization threshold for Fe XIX. Whether this level lies above or below the continuum is an example of the uncertainty in the resonance energies typical for all calculations (see below).

Another example of the uncertainty in the resonance energies is shown by the unresolved near 0 eV \( 2s^22p^3(2D_{5/2})15l \) resonance. Our quantum defect, AUTOSTRUCTURE, and MCDF calculations find that the \( 15i \) is the lowest lying DR resonance for this complex. HULLAC calculates that the \( 15f, g, \) and \( h \) levels are also DR resonances.

Figure 4 shows the ratio of the AUTOSTRUCTURE, HULLAC, and MCDF resonance energies relative to the measured resonance energies. Below 2 eV, agreement between theory and experiment is not that good, with discrepancies between theory and experiment of up to 30%, 35%, and 24% for AUTOSTRUCTURE, HULLAC, and MCDF, respectively. A visual comparison between R-matrix results and experiment finds discrepancies of up to 25% in this energy range. In Figure 5 we compare the theoretical and experimental results. The
AUTOSTRUCTURE, MCDF, and R-matrix results, largely predict the correct resonance strengths. A uniform shift of the theoretical results to lower energies would dramatically improve the agreement between theory and experiment. In the energy range shown, the HULLAC results appear to be correctly predicting some of the DR resonances and miss out on others.

An extreme example of the discrepancies of theoretical with the measured resonance energies is shown by the resonance predicted by AUTOSTRUCTURE, MCDF, and R-matrix (but not HULLAC) calculations to occur at $\approx 0.04$ eV. As discussed in § 2, this resonance probably occurs at an energy below 0.015 eV, contributing to the unresolved, near 0 eV recombination signal. These discrepancies of theory with experiment below 0.8 eV makes DR of Fe XX an excellent case for testing atomic structure calculations on ions with partially filled outer shells.

For energies above 2 eV, AUTOSTRUCTURE and MCDF calculated resonance energies agree with experiment to within 2%. R-matrix energies agree with experiment to within 3%. HULLAC agrees with experiment to within 5%. The relative agreement between theory and experiment improves as the collision energy increases.

Figure 6 shows the ratio of the AUTOSTRUCTURE, HULLAC, and MCDF resonance strengths relative to the measured resonance strengths. We use the data listed in Table 2. The mean value of this ratio is $0.98 \pm 0.30(1\sigma)$ for the AUTOSTRUCTURE results, $0.90 \pm 0.33(1\sigma)$ for the HULLAC results, and $1.02 \pm 0.30(1\sigma)$ for the MCDF results. These results do not change significantly if we leave out of our analysis the weakest 10% of the measured resonances. Our R-matrix results are in good agreement with the AUTOSTRUCTURE results and show similar scatter in the theory-to-experiment ratio of resonance strengths. The mean values all lie within our estimated total experimental error limits. However, the $1\sigma$ standard deviations for these ratios show that a significant number of calculated resonance strengths fall outside the estimated relative experimental uncertainty limits of $\lesssim 10\%$.

Between 0.08 and 1 eV, AUTOSTRUCTURE, HULLAC, MCDF and R-matrix calculations all yield resonance strengths smaller than experiment. The cause of this systematic shift is unlikely to be due to our method for extracting resonance strengths from the experimental results. The spectrum between 0.08 and 1 eV is well resolved and we have a high degree of confidence in the accuracy of the fit to the measured non-resonant background which we subtract out to fit for the DR resonance strengths and energies.

Shown in Figure 7 are the resonance strength ratios for the AUTOSTRUCTURE/MCDF, HULLAC/MCDF, and HULLAC/AUTOSTRUCTURE results. The mean values of these ratios are, respectively, $0.96 \pm 0.10(1\sigma)$, $0.88 \pm 0.26(1\sigma)$, and $0.92 \pm 0.28(1\sigma)$. These results
do not change significantly if we leave out of our analysis those resonances corresponding to the weakest 10% of the measured resonances. Agreement between our AUTOSTRUCTURE and MCDF results is good, much better than it is for either calculation with experiment. Our HULLAC results are in somewhat poorer agreement with our AUTOSTRUCTURE and MCDF calculations.

A comparison between the various theoretical resonance strengths as well as with the experimental results indicates that the HULLAC methodology for calculating DR forming \(2s^22p^3nl\) resonance configurations is incomplete. For example, HULLAC tends to underestimate significantly the \(2s^22p^3(2D_{3/2,5/2})nl\) resonance strengths and to overestimate significantly the \(2s^22p^3(2P_{1/2,3/2})nl\ (l \geq 3)\) resonance strengths. These errors are most likely due to configuration mixings induced by the parametric potential, transferring contributions from one series to another, and to the fact that HULLAC does not include the one-electron operator autoionization transitions in which the initial and final states differ by only one orbital. These interactions can increase or decrease the rate or have no effect at all. Work is underway to modify HULLAC to include the one-electron operator (Bar-Shalom 2001).

Another point of note is that the AUTOSTRUCTURE and MCDF results find a factor of \(\approx 2\) drop between the resonance strength for the \(2s^22p^3(2P_{1/2})21l\ (l \geq 0)\) and the \(2s^22p^3(2P_{1/2})22l\ (l \geq 0)\) levels. This is attributed to the opening up of the \(2s^22p^3(2P_{1/2})nl \rightarrow 2s^22p^3(2D_{5/2})+e^-\) Auger channel which reduces the radiative branching ratio by about a half. HULLAC results predict this Auger channel to open up between the \(2s^22p^3(2P_{1/2})24l\ (l \geq 0)\) and \(2s^22p^3(2P_{1/2})25l\ (l \geq 0)\) resonances.

There are a number of other outstanding discrepancies. Here we only call attention to the most glaring examples. HULLAC underestimates the \(2s^22p^3(2P_{3/2})6d\) resonance strengths between \(\approx 15 - 16\) eV. HULLAC also underestimates the resonance strength for two \(2s^22p^3(2P_{3/2})6f\) resonances at 17.229 and 17.242 eV. AUTOSTRUCTURE underestimates the \(2s^22p^3(2D_{3/2})17d_{3/2}\ (J = 3)\) resonance strength at \(\approx 0.09\) eV by a factor of \(\approx 2\).

5.1. Rate Coefficients

RR calculations have been carried out using R-matrix techniques and topped up using AUTOSTRUCTURE as described above. Arnaud & Raymond (1992) have calculated the rate coefficient for RR of Fe XX and presented a fit to their results which is supposed to be valid between \(10^5\) and \(10^8\) K. Their results are plotted in Figure 3(a). We find that their rate coefficient agrees with our R-matrix results to within 10% for \(k_B T_e\) of between \(\approx 10^{3.4}\) and \(\approx 10^{7.8}\) K.
The calculations of Jacobs et al. (1977) and Roszman (Arnaud & Raymond 1992) were carried out using perturbative techniques, but they only published Maxwellian-averaged rate coefficients. Savin et al. (1999) demonstrated that comparisons of only Maxwellian-averaged rate coefficients cannot be used reliably to distinguish between different theoretical techniques. Disagreement between experiment and theory can be used to demonstrate the inadequacy of a particular theoretical technique. However, agreement between experiment and theory can be fortuitous. A detailed comparison of resonance strengths and energies is the only way to verify the accuracy of DR rate coefficient calculations. Unfortunately, neither Jacobs et al. nor Roszman published their calculated resonance strengths and energies.

Figure 3(a) shows the theoretical $\Delta N = 0$ DR rate coefficients of Jacobs et al. as fitted by Shull & van Steenberg (1982) and of Roszman as reported by Arnaud & Raymond (1992). Fe XX is predicted to peak in fractional abundance in an optically thin, low-density photoionized plasma of cosmic abundances at $k_B T_e \approx 35$ eV (Kallman & Bautista 2001). At this temperature, our experimentally derived DR rate coefficient is a factor of $\approx 1.8$ larger than the rate coefficient of Roszman and of $\approx 4$ times larger than the rate coefficient of Jacobs et al. The reason for these discrepancies is most likely because these calculations did not correctly predict the DR resonance structure at the relevant energies. Also, neither calculation accounts for DR via $2p_{1/2} \rightarrow 2p_{3/2}$ core excitations. The experimentally-derived DR rate coefficient is $\approx 4$ times larger than the RR rate coefficient at $k_B T_e \approx 35$ eV.

We have calculated the $\Delta N = 0$ rate coefficient for DR of Fe XX using our AUTOSTRUCTURE, HULLAC, MCDF, and R-Matrix techniques. The results are shown in Figure 3(b). For $k_B T_e \gtrsim 10$ eV, our experimental and theoretical results agree to better than $\approx 15\%$. This temperature range includes the predicted zone of formation for Fe XX in a photoionized plasma of cosmic abundances. We note that for $k_B T_e \gtrsim 100$ eV, $N = 2 \rightarrow N' = 3$ DR begins to contribute more than 10% to the total DR rate coefficient (Arnaud & Raymond 1992). We plan to measure DR via this core excitation at a future date. Agreement below $k_B T_e \lesssim 1$ eV is difficult to quantify due to current theoretical and experimental limitation for studying resonances near 0 eV.

6. Conclusions

We have measured the resonance strengths and energies for $\Delta N = 0$ DR of Fe XX. The relative experimental uncertainty is estimated at $\lesssim 10\%$ and the total experimental uncertainty at $\lesssim 20\%$. We have also calculated resonance strengths and energies using the state-of-the-art AUTOSTRUCTURE, HULLAC, MCDF, and R-matrix methods. On average we find good agreement between the theoretical and experimental resonance strengths.
However, a large number of the theoretical resonance strengths differ from the measured values by more than three times the relative experimental uncertainty limits. These discrepancies suggest errors in the calculated level populations and line emission spectrum for the recombined ions.

We have used our experimental and theoretical results to produce Maxwellian-averaged rate coefficients for $\Delta N = 0$ DR of Fe XX. For $k_B T_e \gtrsim 10$ eV (which includes the predicted temperature of formation for Fe XX in a photoionized plasma), theory and experiment agree to better than $\approx 15\%$. Apparently many of the discrepancies between the theoretical and experimental resonance strengths average away when one calculates the Maxwellian-averaged rate coefficient.

Agreement for $k_B T_e \lesssim 1$ eV is difficult to quantify due to current theoretical and experimental limitation. Published $L S$-coupling DR rate coefficients are in poor agreement with experiment for $k_B T_e \lesssim 80$ eV. Lastly, we have calculated the rate coefficient for RR of Fe XX. Our RR results are in good agreement with published calculations.

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Table 1. Experimental and (unshifted) theoretical energy levels (relative to the ground state) for the \( n = 2 \) shell of Fe XX.

| Level | Experiment\(^a\) | AUTOSTRUCTURE\(^b,c\) | Bahtia et al.\(^d\) | Donnelly et al.\(^e\) | HULLAC\(^b\) | MCDF\(^b\) | Zhang & Pradhan\(^f\) |
|-------|------------------|-------------------------|---------------------|---------------------|---------------|--------------|---------------------|
| \( 2s^2 2p^3 \quad 4S_3/2 \) | 0               | 0                       | 0                   | 0                   | 0             | 0            | 0                   |
| \( 2s^2 2p^3 \quad 2D_{5/2} \) | 17.1867          | 17.4428                 | 17.5337             | 17.5652             | 17.3514       | 17.4848      | 17.400              |
| \( 2s^2 2p^3 \quad 2D_{3/2} \) | 21.8373          | 22.5928                 | 22.5013             | 22.6023             | 22.4259       | 22.2628      | 21.376              |
| \( 2s^2 2p^3 \quad 2P_{1/2} \) | 32.2694          | 32.1386                 | 32.3219             | 32.4921             | 31.9788       | 32.1682      | 32.245              |
| \( 2s^2 2p^3 \quad 2P_{3/2} \) | 40.0890          | 39.9930                 | 40.2327             | 40.2943             | 40.0720       | 40.0987      | 39.908              |
| \( 2s^2 2p^4 \quad 4P_{5/2} \) | 93.3266          | 92.9521                 | 93.1364             | 93.4356             | 93.4074       | 93.2280      | 93.198              |
| \( 2s^2 2p^4 \quad 4P_{3/2} \) | 101.769          | 101.1239                | 101.429             | 101.5764            | 101.5300      | 101.906      | 101.30              |
| \( 2s^2 2p^4 \quad 4P_{1/2} \) | 104.486          | 103.8390                | 104.154             | 104.2588            | 104.3240      | 104.592      | 103.99              |
| \( 2s^2 2p^4 \quad 2D_{5/2} \) | 129.262          | 130.0774                | 130.2383            | 130.2458            | 130.5768      | 129.635      | 129.91              |
| \( 2s^2 2p^4 \quad 2D_{3/2} \) | 131.220          | 132.2033                | 132.4077            | 132.3882            | 132.5073      | 131.506      | 131.65              |
| \( 2s^2 2p^4 \quad 2S_{1/2} \) | 148.193          | 148.8263                | 149.0889            | 149.1895            | 149.3152      | 148.891      | 148.595             |
| \( 2s^2 2p^4 \quad 2P_{3/2} \) | 154.042          | 155.5766                | 155.9993            | 155.5839            | 156.2177      | 155.532      | 154.967             |
| \( 2s^2 2p^4 \quad 2P_{1/2} \) | 166.144          | 167.3363                | 167.9012            | 167.4207            | 167.9513      | 167.437      | 166.799             |
| \( 2p^5 \quad 2P_{3/2} \)    | 242.330          | 244.6941                | 245.6268            | 244.4497            | 245.6736      | 244.6024     | 243.455             |
| \( 2p^5 \quad 2P_{1/2} \)    | 255.680          | 258.1554                | 259.2832            | 257.8325            | 258.9285      | 257.3803     | 256.768             |

\(^a\)Sugar & Corliss (1985).

\(^b\)Present results.

\(^c\)Also for R-matrix results (see § 4.4.)

\(^d\)Bhatia et al. (1989).

\(^e\)Donnelly et al. (1999).

\(^f\)Zhang & Pradhan (2000).
Table 2. Comparison of the measured and calculated resonance energies $E_d$ and energy-integrated cross sections $S_d$ for Fe XX to Fe XIX $\Delta N = 0$ DR.

| Dominant component | $E_d$ (eV) AUTOSTRUCTURE $^a$ | $S_d$ ($10^{-21}$ cm$^2$ eV) HULLAC$^a$ | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) MCDF$^a$ | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) Experiment$^{b,c}$ | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) AUTOSTRUCTURE | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) HULLAC | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) MCDF | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) Experiment$^b$ |
|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| $2s^2p^3(2D_{5/2})_{17f}^{15f}d,e$ | 4.734E-03 6.407E-02 | 1799.0 373.1 85381 141882.0 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 5.216E-03 9.883E-02 | 2.099E-03 7494.9 $\ll$ 0.1 51801 105417.0 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 5.591E-03 0.1008 | 1.0E-03 3633.4 $\ll$ 0.1 13740 63979.5 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 6.140E-03 0.1008 | 1.8E-03 2072.4 $\ll$ 0.1 664 25492.4 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 6.347E-03 0.1008 | 2.0E-03 1270.4 $\ll$ 0.1 3234 10574.9 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 6.522E-03 0.1008 | 2.2E-03 720.07 $\ll$ 0.1 1688 6862.1 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 6.673E-03 0.1008 | 2.4E-03 326.65 $\ll$ 0.1 735 3049.8 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 6.804E-03 0.1008 | 2.6E-03 101.22 $\ll$ 0.1 405 1756.9 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 0.0576 0.0455 | 0.0030 36208.0 450000.0 | $2s^2p^3(2D_{5/2})_{15k}^{15k}d$ | 0.0576 0.0030 | 0.0030 36100.0 450000.0 |
| $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 2) | 0.0867 0.0954 0.0751 | 1646.7 1070.5 1745.0 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 1) | 0.0905 0.0985 0.0790 | 771.0 240.7 848.3 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 3) | 0.0903 0.1001 0.0794 | 316.0 1123.7 700.6 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 4) | 0.0887 0.1006 0.0810 | 980.4 315.7 1045.0 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 0) | 0.0971 0.1050 0.0861 | 165.9 95.5 184.0 | Blend | 0.0870 0.09842 0.0783 0.0810 ± 0.0002 | 3880.0 2846.1 4522.9 4956.9 ± 96.3 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 3) | 0.0999 0.1098 0.0913 | 2669.0 2005.3 2943.0 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 2) | 0.1099 0.1206 0.1019 | 2096.0 950.1 2048.0 | $2s^2p^3(2D_{3/2})_{17d}^{17d}$ (J = 1) | 0.1165 0.1273 0.1083 | 1029.2 679.4 989.6 | Blend | 0.1065 0.1159 0.0977 0.1019 ± 0.0002 | 5794.2 3634.8 5980.6 8020.0 ± 147.4 | $2s^2p^3(2D_{3/2})_{17f}$ | 0.1750 0.1914 0.1678 0.1690 ± 0.0018 | 2274.3 958.7 2316.8 2873.3 ± 126.7 | $2s^2p^3(2D_{3/2})_{17f}$ (l ≥ 3) | 0.1870 0.2099 0.1839 0.1906 ± 0.0033 | 1565.9 57.2 1277.6 2108.4 ± 225.8 | $2s^2p^3(4P_{3/2})_{7d}^{17f}$ (J = 0) | 0.2919 0.2967 0.2749 | 584.1 588.5 646.3 | $2s^2p^3(4P_{3/2})_{7d}^{17f}$ (J = 1) | 0.2894 0.2997 0.2761 | 1845.8 1715.1 1676.0 | Blend | 0.2900 0.2989 0.2758 0.2248 ± 0.0025 | 2429.9 2303.6 2632.3 3101.8 ± 56.9 | $2s^2p^3(4P_{3/2})_{7d}^{17f}$ (J = 3) | 0.3484 0.2978 ± 0.0002 | 7961.6 9250.4 ± 99.4 |
| Dominant component | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) |
|-------------------|-----------|----------------------|
|                   | AUTOSTRUCTURE $^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE   | HULLAC | MCDF | Experiment$^b$ |
| $2s^2p^3(4s^3/2)7d_{3/2} (J = 3)^d$ | 0.3015 | 0.3444 | 0.2978 ± 0.0002 | 6518.5 | 7089.0 | 9250.4 ± 99.4 |
| $2s^2p^3(4s^3/2)7d_{5/2} (J = 2)$ | 0.4321 | 0.3841 | 0.4306 | 0.3860 ± 0.0004 | 4696.0 | 3699.3 | 4188.0 | 5344.0 ± 91.5 |
| $2s^2p^3(4p^3/2)7p_{3/2} (J = 2)$ | 0.4815 | 0.5088 | 0.4834 | 0.4313 ± 0.0008 | 1810.6 | 1659.1 | 1814.0 | 2289.0 ± 73.0 |
| $2s^2p^3(4s^3/2)7d_{5/2} (J = 1)$ | 0.5382 | 0.4902 | 0.5362 | 0.4955 ± 0.0004 | 3597.9 | 2560.5 | 3040.0 | 4101.6 ± 77.3 |
| $2s^2p^3(4p^3/2)7p_{3/2} (J = 1)$ | 0.7646 | 0.7917 | 0.7621 | 0.7015 ± 0.0011 | 1413.2 | 1023.3 | 1255.0 | 1741.7 ± 64.3 |
| $2s^2p^3(4s^3/2)7f_{5/2} (J = 1)$ | 1.1687 | 1.1100 | 1.1653 | | 257.3 | 322.5 | 238.4 |
| $2s^2p^3(4s^3/2)7f_{5/2} (J = 2)$ | 1.2267 | 1.1679 | 1.2212 | | 842.1 | 1024.5 | 941.0 |
| $2s^2p^3(4s^3/2)7f_{7/2} (J = 5)$ | 1.2407 | 1.1760 | 1.2246 | | 1963.0 | 2523.9 | 2318.0 |
| Blend | 1.2308 | 1.1684 | 1.2196 | 1.1861 ± 0.0012 | 3002.4 | 3870.9 | 3497.4 | 3014.9 ± 153.6 |
| $2s^2p^3(4s^3/2)7f_{5/2} (J = 4)$ | 1.2877 | 1.2278 | 1.2741 | | 1548.3 | 1696.3 | 1731.0 |
| $2s^2p^3(4s^3/2)7f_{5/2} (J = 3)$ | 1.3035 | 1.2405 | 1.2916 | | 1180.7 | 1424.0 | 1356.0 |
| Blend | 1.2945 | 1.2336 | 1.2818 | 1.2361 ± 0.0022 | 2729.0 | 3120.3 | 3087.0 | 2855.1 ± 147.8 |
| $2s^2p^3(4s^3/2)7f_{7/2} (J = 2)$ | 1.3602 | 1.3009 | 1.3501 | | 794.7 | 736.8 | 837.8 |
| $2s^2p^3(4s^3/2)7f_{7/2} (J = 4)$ | 1.3704 | 1.3062 | 1.3542 | | 1453.4 | 1563.1 | 1629.0 |
| $2s^2p^3(4s^3/2)7f_{7/2} (J = 3)$ | 1.4047 | 1.3458 | 1.3934 | | 1101.1 | 1069.4 | 1181.0 |
| Blend | 1.3793 | 1.3176 | 1.3659 | 1.3103 ± 0.0008 | 3349.4 | 3369.3 | 3647.8 | 4025.0 ± 80.5 |
| $2s^2p^3(4s^3/2)7g_{7/2} (J = 2)$ | 1.4342 | 1.3752 | 1.4252 | | 183.35 | 183.3 | 162.2 |
| $2s^2p^3(4s^3/2)7g_{9/2} (J = 3)$ | 1.4545 | 1.3927 | 1.4420 | | 471.6 | 465.4 | 425.1 |
| $2s^2p^3(4s^3/2)7g_{7/2} (J = 5)$ | 1.4587 | 1.4002 | 1.4456 | | 1031.2 | 1059.2 | 1051.0 |
| $2s^2p^3(4s^3/2)7g_{9/2} (J = 6)$ | 1.4705 | 1.4082 | 1.4542 | | 1208.9 | 1272.5 | 1241.0 |
| Blend | 1.4614 | 1.4099 | 1.4476 | 1.4270 ± 0.0009 | 2895.0 | 2980.3 | 2879.3 | 2936.8 ± 94.1 |
| $2s^2p^3(4s^3/2)7g_{7/2} (J = 3, 4)$ | 1.4986 | 1.4471 | 1.4949 | | 1453.0 | 1492.5 | 1466.1 |
| $2s^2p^3(4s^3/2)7l (l \geq 4)$ | 1.5173 | 1.4516 | 1.4985 | | 8848.6 | 9162.2 | 8777.5 |
| $2s^2p^3(4s^3/2)7g_{9/2} (J = 4, 5)$ | 1.5214 | 1.4546 | 1.5020 | | 1798.0 | 1897.6 | 1833.8 |
| Blend | 1.5157 | 1.4515 | 1.4986 | 1.4852 ± 0.0003 | 12100.1 | 12552.3 | 12077.4 | 11738.0 ± 107.9 |
| $2s^2p^3(2D_{5/2}^4)18s (J = 1, 2)$ | 1.6999 | 1.6669 | 1.6731 | 1.6562 ± 0.0063 | 31.6 | 27.7 | 40.8 | 104.6 ± 24.6 |
| $2s^2p^3(2D_{5/2}^4)18p$ | 1.8204 | 1.8212 | 1.8043 | 1.7964 ± 0.0047 | 91.0 | 70.5 | 94.4 | 147.2 ± 25.7 |
| $2s^2p^3(2D_{5/2}^4)18d$ | 1.9505 | 1.9616 | 1.9424 | | 416.4 | 295.3 | 411.8 |
| Dominant component | AUTOSTRUCTURE a | HULLAC a | MCDF a | Experiment b,c | AUTOSTRUCTURE | HULLAC | MCDF | Experiment b |
|--------------------|-----------------|----------|--------|---------------|---------------|---------|------|---------------|
| 2s2p3(2S1/2)6s (J = 1) | 2.0269 | 2.0808 | 1.9620 | 1.9398 ± 0.0022 | 256.8 | 288.7 | 339.7 | |
| Blend | 1.9796 | 2.0205 | 1.9513 | | 673.2 | 584.0 | 751.5 | 703.0 ± 30.4 |
| 2s2p3(2D3/2)18f (l ≥ 3) | 2.0178 | 2.0312 | 2.0120 | | 289.1 | 79.6 | 274.7 | |
| 2s2p3(2D5/2)16s (J = 2, 3) | 2.1845 | 2.2154 | 2.1430 | | 47.9 | 54.2 | 61.9 | |
| Blend | 2.0415 | 2.1058 | 2.0361 | 2.0101 ± 0.0025 | 337.0 | 133.8 | 336.6 | 409.6 ± 30.7 |
| 2s2p3(2P1/2)13s | 2.2733 | 2.3486 | 2.2686 | | 18.6 | 21.8 | 18.8 | |
| 2s2p3(2D3/2)16p | 2.3585 | 2.4070 | 2.3354 | | 134.2 | 120.2 | 132.1 | |
| 2s2p3(2S1/2)6s (J = 0) | 2.4620 | 2.5244 | 2.4147 | | 71.1 | 75.4 | 90.5 | |
| Blend | 2.3943 | 2.4419 | 2.3599 | 2.3264 ± 0.0038 | 205.3 | 217.4 | 241.4 | 254.3 ± 26.9 |
| 2s2p3(2D5/2)16d | 2.5482 | 2.6107 | 2.5358 | 2.5305 ± 0.0017 | 605.7 | 520.0 | 573.4 | 589.0 ± 21.9 |
| 2s2p3(2P1/2)13p1/2 (J = 1) | 2.5758 | 2.6593 | 2.5739 | | 12.2 | 18.0 | 11.1 | |
| 2s2p3(2D3/2)16f | 2.6283 | 2.6975 | 2.6245 | | 273.8 | 265.6 | 277.5 | |
| 2s2p3(2P1/2)13p3/2 (J = 1) | 2.6229 | 2.7096 | 2.6247 | | 23.7 | 18.0 | 24.8 | |
| 2s2p3(2P1/2)13p5/2 (J = 2) | 2.6306 | 2.7174 | 2.6319 | | 31.9 | 25.5 | 33.3 | |
| 2s2p3(2P1/2)7d3/2 (J = 2) | 2.7002 | 2.7144 | 2.6955 | | 433.0 | 380.8 | 434.8 | |
| Blend | 2.7202 | 2.7384 | 2.7224 | | 342.1 | 266.0 | 320.3 | |
| 2s2p3(2D5/2)16f (l ≥ 4) | 2.6466 | 2.7207 | 2.6426 | | 232.1 | 249.8 | 197.8 | |
| 2s2p3(2P1/2)13p1/2 (J = 0) | 2.6512 | 2.7351 | 2.6502 | | 8.0 | 6.3 | 8.8 | |
| 2s2p3(2P1/2)7d5/2 (J = 3) | 2.7864 | 2.7968 | 2.7742 | | 780.0 | 633.7 | 752.3 | |
| Blend | 2.7535 | 2.7750 | 2.7459 | 2.7131 ± 0.0009 | 1020.1 | 889.8 | 958.9 | 827.9 ± 22.8 |
| 2s2p3(2P1/2)13d | 2.9803 | 3.0716 | 2.9883 | 2.9826 ± 0.0018 | 340.4 | 270.4 | 325.8 | 304.9 ± 17.1 |
| 2s2p3(2P1/2)13l (l ≥ 3) | 3.1745 | 3.2693 | 3.1710 | | 144.1 | 351.0 | 134.5 | |
| 2s2p3(2P1/2)7d5/2 (J = 2) | 3.2834 | 3.3013 | 3.2749 | | 853.59 | 552.7 | 735.5 | |
| 2s2p3(2D3/2)19a (J = 1, 2) | 3.3028 | 3.2811 | 3.2796 | | 13.8 | 11.9 | 17.7 | |
| Blend | 3.2682 | 3.2419 | 3.2593 | 3.2214 ± 0.0012 | 1011.5 | 915.6 | 887.7 | 926.4 ± 22.0 |
| 2s2p3(2D3/2)19p | 3.4051 | 3.3988 | 3.3895 | 3.3934 ± 0.0021 | 41.1 | 31.1 | 42.8 | 25.1 ± 13.1 |
Table 2—Continued

| Dominant component | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) |
|--------------------|------------|-------------------------------|
|                    | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
| $2s^22p^3(2D_{5/2}^0)^{19}d$ | 3.5157 | 3.5189 | 3.5080 | 3.5102 ± 0.0038 | 196.3 | 136.0 | 194.5 | 202.9 ± 19.3 |
| $2s^22p^3(2D_{5/2}^0)^{19}f$ ($l \geq 3$) | 3.5734 | 3.5791 | 3.5660 | 3.5704 ± 0.0055 | 137.0 | 37.3 | 134.1 | 147.2 ± 22.2 |
| $2s^22p^3(4P_{1/2})7f_{5/2}$ ($J = 2$) | 3.9787 | 3.9882 | 3.9714 | | 281.1 | 323.0 | 321.5 | |
| $2s^22p^3(4P_{1/2})7f_{7/2}$ ($J = 3$) | 3.9867 | 3.9936 | 3.9745 | | 390.4 | 454.5 | 448.6 | |
| $2s^22p^3(4P_{1/2})7f_{7/2}$ ($J = 4$) | 4.0096 | 4.0128 | 3.9923 | | 491.8 | 560.9 | 562.1 | |
| Blend | 3.9945 | 4.0003 | 3.9813 | 3.9390 ± 0.0010 | 1163.3 | 1338.4 | 1332.2 | 1024.2 ± 16.8 |
| $2s^22p^3(4P_{1/2})7f_{7/2}$ ($J = 3$) | 4.1012 | 4.1122 | 4.0894 | 4.0319 ± 0.0021 | 378.8 | 317.6 | 395.1 | 379.7 ± 19.1 |
| $2s^22p^3(4P_{1/2})7f_{7/2}$ ($J = 4$) | 4.2149 | 4.2254 | 4.2035 | 4.1861 ± 0.0003 | 3006.6 | 3014.7 | 3023.7 | 2722.2 ± 20.9 |
| $2s^22p^3(2D_{5/2}^0)^{17}s$ | 4.4533 | 4.4823 | 4.4200 | 4.3832 ± 0.0201 | 19.4 | 22.0 | 25.0 | 39.2 ± 15.2 |
| $2s^22p^3(2D_{5/2}^0)^{17}p$ | 4.5982 | 4.6427 | 4.5787 | 4.5872 ± 0.0140 | 57.0 | 53.1 | 56.3 | 52.0 ± 15.1 |
| $2s^22p^3(2D_{5/2}^0)^{20}p$ | 4.7568 | 4.7317 | 4.7457 | | 25.1 | 18.6 | 26.2 | |
| $2s^22p^3(2D_{5/2}^0)^{17}d$ | 4.7561 | 4.8011 | 4.7578 | | 270.4 | 232.8 | 256.0 | |
| $2s^22p^3(2P_{3/2}^0)^{12}s$ ($J = 1, 2$) | 4.6396 | 4.7712 | 4.7820 | | 24.4 | 24.1 | 23.3 | |
| Blend | 4.7496 | 4.7938 | 4.7591 | 4.7537 ± 0.0030 | 319.9 | 275.5 | 305.4 | 204.2 ± 13.5 |
| $2s^22p^3(2D_{5/2}^0)^{17}l$ ($l \geq 3$) | 4.8323 | 4.8887 | 4.8254 | | 220.3 | 234.8 | 217.7 | |
| $2s^22p^3(2D_{5/2}^0)^{20}l$ ($l \geq 2$) | 4.8718 | 4.8410 | 4.8649 | | 206.6 | 101.6 | 205.5 | |
| Blend | 4.8514 | 4.8743 | 4.8446 | 4.8490 ± 0.0022 | 426.9 | 336.4 | 422.7 | 457.1 ± 17.9 |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{1/2}$ ($J = 1$) | 5.1934 | 5.1852 | 5.1924 | | 15.2 | 12.3 | 16.3 | |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{1/2}$ ($J = 3$) | 5.2155 | 5.2096 | 5.2163 | | 4.4 | 14.4 | 6.9 | |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{1/2}$ ($J = 2$) | 5.2194 | 5.2102 | 5.2171 | | 18.7 | 19.0 | 21.3 | |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{3/2}$ ($J = 1$) | 5.2312 | 5.2244 | 5.2314 | | 13.9 | 11.8 | 14.5 | |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{3/2}$ ($J = 2$) | 5.2551 | 5.2498 | 5.2570 | | 23.0 | 16.9 | 24.5 | |
| $2s^22p^3(2S_{1/2})^6p_{1/2}$ ($J = 0$) | 5.3722 | 5.4509 | 5.3409 | | 10.2 | 14.0 | 15.1 | |
| Blend | 5.2444 | 5.2542 | 5.2445 | 5.2589 ± 0.0050 | 85.4 | 88.4 | 98.8 | 83.0 ± 8.6 |
| $2s^22p^3(2P_{3/2}^0)^{12}p_{3/2}$ ($J = 0$) | 5.3694 | 5.3629 | 5.3724 | | 4.9 | 3.7 | 5.1 | |
| $2s^22p^3(2S_{1/2})^6p_{1/2}$ ($J = 1$) | 5.5090 | 5.5892 | 5.4728 | | 119.2 | 125.4 | 126.0 | |
| Blend | 5.5037 | 5.5827 | 5.4697 | 5.4383 ± 0.0031 | 124.1 | 129.1 | 131.1 | 92.4 ± 6.9 |
| $2s^22p^3(2P_{3/2}^0)^{12}d$ | 5.7194 | 5.7103 | 5.7154 | 5.7240 ± 0.0019 | 382.7 | 316.8 | 391.4 | 366.6 ± 15.2 |
Table 2—Continued

| Dominant component | \( E_d \) (eV) | \( S_d \) (10\(^{-21}\) cm\(^2\) eV) |
|---------------------|----------------|---------------------------------|
| 2s\(^2\)p\(^2\)(2\(S\)\(_{1/2}\))6p\(_{3/2}\) (\( J = 2 \)) | 5.7870 | 151.8 |
| 2s\(^2\)p\(^2\)(2\(D\)\(_{3/2}\))21s (\( J = 1, 2 \)) | 5.8433 | 5.7 |
| Blend | 5.7890 | 5.7890 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))21p | 5.9189 | 17.4 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{3/2}\))12f | 5.9359 | 65.7 |
| Blend | 5.9323 | 83.1 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{1/2}\))12l (\( J = 1 \)) | 5.9565 | 44.5 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))21l (\( J = 2 \)) | 6.0182 | 144.0 |
| Blend | 6.0029 | 192.3 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))18s (\( J = 2, 3 \)) | 6.3507 | 11.4 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))18p | 6.4726 | 33.9 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{3/2}\))14s | 6.4642 | 5.2 |
| Blend | 6.4715 | 39.1 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))18l (\( J = 2 \)) | 6.6342 | 296.4 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{1/2}\))14p | 6.7424 | 23.4 |
| Blend | 6.6421 | 319.8 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))22l (\( J \geq 0 \)) | 7.0023 | 120.0 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{1/2}\))14d | 7.0360 | 115.2 |
| Blend | 7.0188 | 235.2 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{1/2}\))14f (\( J \geq 3 \)) | 7.1840 | 50.0 |
| 2s\(^2\)p\(^3\)(2\(P\)\(_{3/2}\))6s (\( J = 1, 2 \)) | 7.9915 | 211.8 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{3/2}\))23l (\( J \geq 0 \)) | 7.8658 | 96.4 |
| Blend | 7.9522 | 308.2 |
| 2s\(^2\)p\(^3\)(2\(D\)\(_{5/2}\))19f (\( J \geq 0 \)) | 8.1732 | 233.9 |
| Dominant component | AUTOSTRUCTURE $^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
|--------------------|-------------------|-------------|---------|---------------------|---------------|---------|------|----------------|
| $s^2p^3(2D_{rac{5}{2}}^{o})24l$ ($l \geq 0$) | 8.6277 | 8.5996 | 8.6206 | 8.6581 ± 0.0054 | 77.2 | 30.6 | 78.4 | 72.3 ± 8.8 |
| $2s^2p^3(2D_{rac{5}{2}}^{o})25l$ ($l \geq 0$) | 9.2999 | 9.4499 | 9.2932 | | 63.2 | 20.3 | 64.2 | |
| $2s^2p^3(2P_{rac{1}{2}}^{o})6d_{3/2}$ ($J = 1$) | 9.3639 | 9.4735 | 9.3673 | | 94.9 | 103.9 | 103.0 | |
| $2s^2p^3(2P_{rac{1}{2}}^{o})6d_{3/2}$ ($J = 2$) | 9.4730 | 9.5652 | 9.4567 | | 205.6 | 178.8 | 195.0 | |
| $2s^2p^3(2D_{rac{5}{2}}^{o})20l$ ($l \leq 2$) | 9.4902 | 9.4873 | 9.4659 | | 105.5 | 88.8 | 102.0 | |
| $2s^2p^3(2P_{rac{1}{2}}^{o})6d_{3/2}$ ($J = 3$) | 9.4961 | 9.5760 | 9.4703 | | 271.1 | 247.3 | 266.0 | |
| Blend | 9.4537 | 9.5400 | 9.4360 | 9.4117 ± 0.0023 | 740.3 | 639.1 | 730.2 | 666.6 ± 15.1 |
| $2s^2p^3(2D_{rac{5}{2}}^{o})20l$ ($l \geq 3$) | 9.5526 | 9.5784 | 9.5457 | 9.5853 ± 0.0064 | 66.1 | 68.6 | 67.6 | 65.0 ± 13.3 |
| $2s^2p^3(2P_{rac{1}{2}}^{o})15s$ | 9.8746 | 9.8758 | 9.8303 | | 2.6 | 3.3 | 2.8 | |
| $2s^2p^3(2P_{rac{1}{2}}^{o})26l$ ($l \leq 1$) | 9.8425 | 9.9739 | 9.8322 | | 7.2 | 2.8 | 8.0 | |
| $2s^2p^3(2P_{rac{1}{2}}^{o})6d_{3/2}$ ($J = 2$) | 9.8623 | 9.9524 | 9.8457 | | 45.9 | 47.1 | 34.1 | |
| Blend | 9.8603 | 9.9488 | 9.8423 | 9.7502 ± 0.0162 | 55.7 | 53.2 | 44.9 | 59.1 ± 10.9 |
| $2s^2p^3(2D_{rac{5}{2}}^{o})26l$ ($l \geq 2$) | 9.9043 | 10.052 | 9.8995 | 9.9212 ± 0.0162 | 45.5 | 13.7 | 45.7 | 53.1 ± 11.2 |
| $2s^2p^3(2P_{rac{1}{2}}^{o})15p$ | 10.083 | 10.105 | 10.060 | | 12.6 | 11.7 | 13.2 | |
| $2s^2p^3(2P_{rac{3}{2}}^{o})13s$ ($J = 1, 2$) | 10.092 | 10.198 | 10.085 | | 8.7 | 8.8 | 9.0 | |
| Blend | 10.087 | 10.145 | 10.070 | 10.101 ± 0.029 | 21.3 | 20.5 | 22.2 | 21.0 ± 14.3 |
| $2s^2p^3(2P_{rac{1}{2}}^{o})15d$ | 10.298 | 10.345 | 10.296 | 10.315 ± 0.012 | 63.7 | 51.8 | 61.7 | 33.9 ± 11.8 |
| $2s^2p^3(2P_{rac{1}{2}}^{o})15l$ ($l \geq 3$) | 10.434 | 10.475 | 10.415 | | 27.5 | 69.1 | 27.3 | |
| $2s^2p^3(2D_{rac{5}{2}}^{o})27l$ ($l \geq 0$) | 10.427 | 10.558 | 10.421 | | 44.7 | 14.0 | 45.4 | |
| $2s^2p^3(2P_{rac{3}{2}}^{o})13p$ | 10.441 | 10.554 | 10.440 | | 31.3 | 30.2 | 35.7 | |
| $2s^2p^3(2D_{rac{5}{2}}^{o})21s(J = 2, 3)$ | 10.494 | 10.496 | 10.475 | | 4.3 | 4.1 | 5.5 | |
| Blend | 10.436 | 10.506 | 10.428 | 10.470 ± 0.006 | 107.8 | 117.4 | 113.9 | 138.6 ± 16.8 |
| $2s^2p^3(2D_{rac{5}{2}}^{o})21l$ ($l \geq 1$) | 10.662 | 10.686 | 10.647 | 10.711 ± 0.028 | 127.7 | 96.4 | 130.0 | 134.7 ± 70.4 |
| $2s^2p^3(2P_{rac{3}{2}}^{o})13l$ ($l \geq 2$) | 10.846 | 11.024 | 10.844 | | 185.7 | 247.7 | 196.0 | |
| $2s^2p^3(2D_{rac{5}{2}}^{o})28l$ ($l \geq 0$) | 10.902 | 11.019 | 10.896 | | 38.3 | 12.3 | 38.9 | |
| Blend | 10.856 | 11.024 | 10.852 | 10.881 ± 0.026 | 224.0 | 260.0 | 234.9 | 213.6 ± 72.5 |
| Dominant component | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
|-------------------|---------------|--------|-----|---------------------|---------------|--------|-----|---------------|
| $2s^2p^4(^2P_{3/2})6p_{1/2}$ ($J = 2$) | 11.208 | 11.278 | 11.169 | 11.099 ± 0.004 | 135.8 | 145.6 | 142.0 | 120.8 ± 12.7 |
| $2s^2p^4(^2P_{3/2})6f$ | 11.328 | 11.414 | 11.323 | | 33.2 | 10.4 | 33.7 | |
| $2s^2p^4(^2P_{1/2})6f$ | 11.435 | 11.508 | 11.406 | | 579.7 | 605.5 | 631.0 | |
| $2s^2p^4(^2P_{3/2})6p_{1/2}$ ($J = 1$) | 11.495 | 11.569 | 11.459 | | 9.1 | 16.5 | 15.9 | |
| $2s^2p^4(^2D_{5/2})22l$ ($l \leq 1$) | 11.561 | 11.585 | 11.544 | | 13.6 | 7.9 | 14.6 | |
| $2s^2p^4(^2P_{3/2})6p_{3/2}$ ($J = 2$) | 11.555 | 11.659 | 11.550 | | 111.9 | 110.6 | 119.0 | |
| $2s^2p^4(^2P_{3/2})6p_{3/2}$ ($J = 3$) | 11.586 | 11.698 | 11.579 | | 62.6 | 61.8 | 58.9 | |
| Blend | 11.461 | 11.544 | 11.437 | 11.435 ± 0.001 | 810.1 | 812.7 | 873.1 | 683.9 ± 11.9 |
| $2s^2p^4(^2D_{5/2})22l$ ($l \geq 2$) | 11.665 | 11.687 | 11.659 | | 91.0 | 72.4 | 89.2 | |
| $2s^2p^4(^2P_{1/2})6g$ | 11.704 | 11.783 | 11.677 | | 450.7 | 461.5 | 464.0 | |
| $2s^2p^4(^2P_{1/2})6h$ | 11.736 | 11.812 | 11.706 | | 267.4 | 274.4 | 280.0 | |
| $2s^2p^4(^2D_{5/2})30l$ ($l \geq 0$) | 11.713 | 11.818 | 11.707 | | 29.0 | 9.1 | 29.4 | |
| $2s^2p^4(^2P_{3/2})6p_{3/2}$ ($J = 0$) | 11.808 | 11.922 | 11.808 | | 1.2 | 1.6 | 1.9 | |
| Blend | 11.710 | 11.785 | 11.685 | 11.749 ± 0.001 | 839.3 | 819.0 | 864.5 | 794.9 ± 11.1 |
| $2s^2p^4(^2D_{5/2})31l$ ($l \geq 0$) | 12.061 | 12.158 | 12.056 | | 25.5 | 8.0 | 25.9 | |
| $2s^2p^4(^2P_{3/2})6p_{3/2}$ ($J = 1$) | 12.261 | 12.376 | 12.260 | | 77.9 | 84.4 | 82.8 | |
| Blend | 12.212 | 12.357 | 12.211 | 12.172 ± 0.009 | 103.4 | 92.4 | 108.7 | 88.2 ± 10.5 |
| $2s^2p^4(^2D_{5/2})32l$ ($l \geq 0$) | 12.664 | 12.468 | 12.371 | | 20.1 | 7.1 | 22.9 | |
| $2s^2p^4(^2P_{3/2})8s$ ($J = 3$) | 12.466 | 12.525 | 12.435 | | 32.2 | 46.4 | 46.7 | |
| $2s^2p^4(^2D_{5/2})23l$ ($l \geq 0$) | 12.520 | 12.541 | 12.511 | | 85.0 | 65.2 | 84.7 | |
| $2s^2p^4(^2P_{3/2})16s$ ($J = 0, 1$) | 12.618 | 12.617 | 12.581 | | 1.7 | 2.1 | 1.8 | |
| Blend | 12.530 | 12.532 | 12.469 | 12.539 ± 0.009 | 139.0 | 120.8 | 156.1 | 168.2 ± 16.7 |
| $2s^2p^4(^2D_{5/2})33l$ ($l \geq 0$) | 12.664 | 12.749 | 12.659 | | 20.1 | 6.3 | 20.3 | |
| $2s^2p^4(^2P_{3/2})8s$ ($J = 2$) | 12.749 | 12.814 | 12.721 | | 35.1 | 32.9 | 42.5 | |
| $2s^2p^4(^2P_{1/2})16p$ | 12.789 | 12.806 | 12.770 | | 8.1 | 7.5 | 8.5 | |
| Blend | 12.727 | 12.804 | 12.709 | 12.787 ± 0.011 | 63.3 | 46.7 | 71.3 | 50.9 ± 13.8 |
| $2s^2p^4(^2D_{5/2})34l$ ($l \geq 0$) | 12.926 | 13.006 | 12.922 | | 18.0 | 5.7 | 18.2 | |
| $2s^2p^4(^2P_{1/2})16p$ ($l \geq 2$) | 13.003 | 13.063 | 12.995 | | 58.3 | 78.3 | 58.1 | |
| Dominant component | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) |
|--------------------|------------|-----------------------------|
| Blend              | 12.985     | 76.3                        |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)35f ($l \geq 0$) | 13.167 | 16.2 |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)24f ($l \geq 0$) | 13.281 | 70.4 |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)36f ($l \geq 0$) | 13.387 | 14.7 |
| Blend              | 13.278     | 101.3                       |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)37f ($l \geq 0$) | 13.590 | 13.3 |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)38f ($l \geq 0$) | 13.777 | 12.1 |
| 2s$^2$p$^4$(4 $P_{3/2}^o$)8$p_{1/2}$ ($J = 2, 3$) | 13.892 | 79.3 |
| Blend              | 13.877     | 91.4                        |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)25f ($l \geq 0$) | 13.953 | 59.1 |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)39f ($l \geq 0$) | 13.950 | 11.1 |
| 2s$^2$p$^4$(4 $P_{3/2}^o$)8$p_{1/2}$ ($J = 4$) | 14.031 | 53.9 |
| 2s$^2$p$^4$(4 $P_{3/2}^o$)8$p_{1/2}$ ($J = 3$) | 14.105 | 96.7 |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)40f ($l \geq 0$) | 14.110 | 10.1 |
| Blend              | 14.042     | 230.9                       |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)41f ($l \geq 0$) | 14.258 | 9.3  |
| 2s$^2$p$^3$(2 $P_{3/2}^o$)14s       | 14.283 | 4.9  |
| 2s$^2$p$^4$(4 $P_{3/2}^o$)8$p_{1/2}$ ($J = 1$) | 14.280 | 50.4 |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)42f ($l \geq 0$) | 14.396 | 8.6  |
| 2s$^2$p$^4$(4 $P_{3/2}^o$)8$p_{1/2}$ ($J = 2$) | 14.407 | 78.6 |
| Blend              | 14.351     | 151.8                       |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)26f ($l \geq 0$) | 14.459 | 50.3 |
| 2s$^2$p$^3$(2 $P_{3/2}^o$)14p       | 14.562 | 17.8 |
| 2s$^2$p$^3$(2 $D_{5/2}^o$)43f ($l \geq 0$) | 14.525 | 7.9  |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)44f ($l \geq 0$) | 14.644 | 7.3  |
| Blend              | 14.558     | 83.3                        |
| 2s$^2$p$^3$(2 $D_{3/2}^o$)nl ($n = 45 - 47$, $l \geq 0$) | 14.857 | 19.0 |
| 2s$^2$p$^3$(2 $P_{1/2}^o$)17s       | 14.887 | 1.2  |
| 2s$^2$p$^3$(2 $P_{1/2}^o$)17s       | 14.887 | 1.2  |
Table 2—Continued

| Dominant component | AUTOSTRUCTURE | HULLAC | MCDF | Experiment<sup>b,c</sup> | AUTOSTRUCTURE | HULLAC | MCDF | Experiment<sup>b</sup> |
|--------------------|---------------|--------|------|-----------------------------|---------------|--------|------|-----------------------------|
| 2s<sup>2</sup>2p<sup>3</sup>(2P<sub>3/2</sub>)14d | 14.865 | 14.966 | 14.861 | 91.7 | 75.5 | 95.4 |
| 2s<sup>2</sup>2p<sup>3</sup>(2P<sub>3/2</sub>)14f (l ≥ 3) | 15.002 | 15.115 | 14.998 | 17.0 | 68.9 | 18.5 |
| 2s<sup>2</sup>2p<sup>3</sup>(2P<sub>1/2</sub>)17p | 15.029 | 15.042 | 15.013 | 5.7 | 6.6 | 6.0 |
| Blend | 14.888 | 15.030 | 14.885 | 14.936 ± 0.008 | 134.6 | 158.8 | 140.5 | 296.2 ± 12.5 |
| 2s<sup>2</sup>2p<sup>3</sup>(2D<sub>5/2</sub>)27l (l ≥ 0) | 15.079 | 15.247 | 15.072 | 43.3 | 24.0 | 43.2 |
| 2s<sup>2</sup>2p<sup>3</sup>(2P<sub>3/2</sub>)6d<sub>5/2</sub> (J = 3) | 15.109 | 15.190 | 15.087 | 157.2 | 30.1 | 159.0 |
| 2s<sup>2</sup>2p<sup>3</sup>(2D<sub>5/2</sub>)ml (n = 48−49, l ≥ 0) | 15.092 | 15.128 | 15.092 | 10.6 | 3.4 | 10.8 |
| 2s<sup>2</sup>2p<sup>3</sup>(2P<sub>1/2</sub>)17l (l ≥ 2) | 15.208 | 15.258 | 15.200 | 41.5 | 74.2 | 41.4 |
| Blend | 15.119 | 15.237 | 15.103 | 15.094 ± 0.005 | 252.6 | 131.7 | 254.4 | 326.2 ± 13.3 |
| 2s<sup>2</sup>2p<sup>4</sup>(2P<sub>3/2</sub>)6d<sub>3/2</sub> (J = 2) | 15.232 | 15.318 | 15.217 | 126.0 | 26.0 | 122.0 |
| 2s<sup>2</sup>2p<sup>3</sup>(2D<sub>5/2</sub>)ml (n = 50−52, l ≥ 0) | 15.290 | 15.323 | 15.290 | 13.6 | 4.4 | 13.8 |
| 2s<sup>2</sup>2p<sup>4</sup>(2P<sub>3/2</sub>)6d<sub>3/2</sub> (J = 3) | 15.327 | 15.427 | 15.312 | 146.2 | 76.6 | 155.0 |
| 2s<sup>2</sup>2p<sup>4</sup>(2P<sub>3/2</sub>)6d<sub>3/2</sub> (J = 4) | 15.350 | 15.437 | 15.322 | 169.7 | 58.8 | 181.0 |
| Blend | 15.308 | 15.411 | 15.290 | 15.290 ± 0.003 | 455.5 | 165.8 | 471.8 | 404.6 ± 10.5 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>3/2</sub> (J = 4) | 15.432 | 15.508 | 15.419 | 74.2 | 76.7 | 77.6 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>3/2</sub> (J = 3) | 15.430 | 15.510 | 15.423 | 58.5 | 60.7 | 61.3 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>3/2</sub> (J = 1) | 15.449 | 15.538 | 15.440 | 65.3 | 13.3 | 56.4 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>3/2</sub> (J = 2) | 15.475 | 15.557 | 15.472 | 42.8 | 43.9 | 44.6 |
| 2s<sup>2</sup>2p<sup>4</sup>(2D<sub>5/2</sub>)ml (n = 53−55, l ≥ 0) | 15.496 | 15.524 | 15.494 | 11.3 | 3.7 | 11.5 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>5/2</sub> (J = 5) | 15.536 | 15.611 | 15.520 | 92.5 | 93.7 | 96.6 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>5/2</sub> (J = 4) | 15.538 | 15.621 | 15.537 | 26.6 | 26.6 | 27.3 |
| 2s<sup>2</sup>2p<sup>4</sup>(2D<sub>5/2</sub>)28l (l ≥ 0) | 15.554 | 15.709 | 15.547 | 37.7 | 20.9 | 37.5 |
| 2s<sup>2</sup>2p<sup>4</sup>(2P<sub>3/2</sub>)6d<sub>3/2</sub> (J = 0) | 15.634 | 15.715 | 15.614 | 8.0 | 1.5 | 5.3 |
| Blend | 15.485 | 15.566 | 15.475 | 15.522 ± 0.003 | 416.9 | 341.0 | 418.1 | 405.3 ± 8.8 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>3/2</sub> (J = 4) | 15.733 | 15.814 | 15.721 | 71.7 | 66.5 | 71.5 |
| 2s<sup>2</sup>2p<sup>4</sup>(2D<sub>5/2</sub>)ml (n = 56−62, l ≥ 0) | 15.758 | 15.782 | 15.756 | 19.9 | 6.5 | 20.3 |
| 2s<sup>2</sup>2p<sup>4</sup>(2P<sub>3/2</sub>)6d<sub>5/2</sub> (J = 1) | 15.857 | 15.936 | 15.832 | 59.8 | 17.5 | 52.8 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>5/2</sub> (J = 0) | 15.912 | 15.988 | 15.900 | 21.6 | 15.7 | 18.7 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>5/2</sub> (J = 3) | 15.956 | 16.036 | 15.943 | 174.8 | 124.0 | 149.0 |
| 2s<sup>2</sup>2p<sup>4</sup>(4P<sub>3/2</sub>)8d<sub>5/2</sub> (J = 1) | 15.962 | 16.039 | 15.949 | 79.3 | 55.8 | 67.6 |
| Blend | 15.894 | 15.970 | 15.875 | 15.813 ± 0.008 | 427.1 | 286.0 | 379.9 | 470.8 ± 45.7 |
Table 2—Continued

| Dominant component | $E_d$ (eV) | $S_d$ (10$^{-21}$ cm$^2$ eV) |
|--------------------|------------|-----------------------------|
|                    | AUTOSTRUCTURE $^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
| $2s^2p^4(2P_{3/2})6d_{5/2} (J = 2)$ | 15.989 | 16.064 | 15.953 | 292.8 | 90.8 | 268.0 |
| $2s^2p^4(2P_{3/2})29l (l \geq 0)$ | 15.986 | 16.124 | 15.974 | 29.3 | 18.3 | 32.8 |
| $2s^2p^4(4P_{3/2})8d_{5/2} (J = 2)$ | 16.003 | 16.083 | 15.992 | 152.2 | 105.4 | 128.0 |
| $2s^2p^4(2D_{5/2})nl (n = 63 - 71, l \geq 0)$ | 16.075 | 16.094 | 16.073 | 17.2 | 5.6 | 17.5 |
| Blend | 15.996 | 16.079 | 15.970 | 15.992 ± 0.004 | 491.5 | 220.1 | 446.3 | 474.2 ± 40.6 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 4)$ | 16.356 | 16.425 | 16.338 | 80.5 | 96.5 | 89.5 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 5)$ | 16.366 | 16.433 | 16.346 | 100.5 | 120.8 | 112.0 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 3)$ | 16.368 | 16.439 | 16.353 | 59.2 | 69.2 | 64.8 |
| $2s^2p^3(2D_{5/2})30l (l \geq 0)$ | 16.365 | 16.499 | 16.360 | 29.1 | 16.1 | 28.9 |
| $2s^2p^4(2D_{5/2})nl (n = 72 - 85, l \geq 0)$ | 16.369 | 16.382 | 16.366 | 16.4 | 5.3 | 16.8 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 2)$ | 16.394 | 16.466 | 16.382 | 33.5 | 37.9 | 35.5 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 6)$ | 16.427 | 16.494 | 16.405 | 119.8 | 139.0 | 132.0 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 1)$ | 16.435 | 16.497 | 16.413 | 5.6 | 6.9 | 5.7 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 0)$ | 16.446 | 16.518 | 16.435 | 0.1 | 0.2 | 0.2 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 4)$ | 16.455 | 16.529 | 16.439 | 81.0 | 71.3 | 80.9 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (J = 5)$ | 16.478 | 16.536 | 16.444 | 101.0 | 101.1 | 105.0 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 3)$ | 16.478 | 16.551 | 16.462 | 58.7 | 52.1 | 58.2 |
| Blend | 16.412 | 16.481 | 16.393 | 16.404 ± 0.004 | 685.4 | 716.4 | 729.5 | 703.9 ± 36.5 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 2)$ | 16.507 | 16.579 | 16.491 | 37.4 | 35.3 | 37.0 |
| $2s^2p^4(4P_{3/2})8f_{7/2} (J = 1)$ | 16.526 | 16.598 | 16.511 | 22.7 | 22.3 | 22.5 |
| $2s^2p^4(4P_{3/2})8f_{5/2} (I \geq 4)$ | 16.561 | 16.632 | 16.544 | 1672.5 | 1386.0 | 1680.0 |
| $2s^2p^4(2D_{5/2})nl (n = 86 - 120, l \geq 0)$ | 16.680 | 16.688 | 16.685 | 18.6 | 6.1 | 18.1 |
| $2s^2p^4(2D_{5/2})31l (l \geq 0)$ | 16.713 | 16.838 | 16.707 | 25.8 | 14.3 | 25.6 |
| $2s^2p^4(2D_{5/2})18l (l \leq 1)$ | 16.901 | 16.880 | 16.866 | 3.8 | 4.9 | 5.4 |
| Blend | 16.564 | 16.633 | 16.547 | 16.585 ± 0.015 | 1780.8 | 1468.9 | 1788.6 | 1766.2 ± 44.4 |
| $2s^2p^4(2D_{5/2})32l (l \geq 0)$ | 17.029 | 17.145 | 17.022 | 23.0 | 12.8 | 22.9 |
| $2s^2p^4(2D_{5/2})18l (l \geq 2)$ | 17.054 | 17.090 | 17.047 | 31.1 | 40.4 | 31.0 |
| $2s^2p^4(2P_{3/2})6f_{7/2} (J = 4)$ | 17.157 | 17.229 | 17.122 | 172.2 | 39.7 | 195.0 |
| $2s^2p^4(2P_{3/2})6f_{5/2} (J = 3)$ | 17.159 | 17.242 | 17.134 | 135.8 | 32.9 | 151.0 |
| Blend | 17.141 | 17.179 | 17.115 | 17.077 ± 0.003 | 362.1 | 125.8 | 399.9 | 256.5 ± 8.6 |
Table 2—Continued

| Dominant component | AUTOSTRUCTURE a | HULLAC b | MCDF a | Experiment b,c | AUTOSTRUCTURE | HULLAC | MCDF | Experiment b |
|--------------------|-----------------|--------|-------|---------------|--------------|--------|--------|---------------|
| 2s2p^3(2P_3/2)6f_5/2 (J = 2) | 17.230 | 17.315 | 17.210 | 21.5 | 23.7 | 96.1 |
| 2s2p^3(2P_3/2)6f_5/2 (J = 4) | 17.299 | 17.386 | 17.274 | 41.3 | 47.5 | 50.3 |
| 2s2p^3(2P_3/2)6f_7/2 (J = 3) | 17.304 | 17.384 | 17.277 | 35.4 | 38.4 | 41.8 |
| 2s2p^3(2P_3/2)6f_7/2 (J = 5) | 17.336 | 17.411 | 17.299 | 36.9 | 42.0 | 45.9 |
| 2s^22p^3(2D_5/2)_3M (l ≥ 0) | 17.316 | 17.425 | 17.310 | 11.3 | 11.5 | 11.4 |
| 2s2p^3(2P_3/2)6f_5/2 (J = 1) | 17.394 | 17.481 | 17.377 | 42.1 | 45.3 | 44.9 |
| 2s2p^3(2P_3/2)6f_7/2 (J = 2) | 17.454 | 17.534 | 17.428 | 42.7 | 42.6 | 46.2 |
| Blend | 17.346 | 17.427 | 17.300 | 17.312 ± 0.007 | 231.2 | 251.0 | 336.6 | 156.5 ± 8.8 |
| 2s2p^3(2P_3/2)6f (l ≥ 4) | 17.555 | 17.640 | 17.553 | 268.9 | 288.5 | 308 |
| 2s2p^3(2P_3/2)4f (l ≥ 0) | 17.575 | 17.681 | 17.572 | 10.2 | 10.4 | 10.3 |
| Blend | 17.566 | 17.641 | 17.554 | 17.544 ± 0.003 | 279.1 | 298.9 | 318.3 | 312.2 ± 10.0 |
| 2s^22p^3(2D_5/2)_3M (l ≥ 0) | 17.818 | 17.915 | 17.812 | 9.2 | 9.4 | 9.9 |
| 2s^22p^3(2P_3/2)_15l (l ≤ 1) | 17.866 | 17.910 | 17.846 | 5.2 | 5.5 | 8.3 |
| 2s^22p^3(2D_5/2)_36l (l ≥ 0) | 18.039 | 18.130 | 18.043 | 8.4 | 8.5 | 9.1 |
| Blend | 17.910 | 17.992 | 17.899 | 17.724 ± 0.061 | 22.8 | 23.4 | 27.3 | 63.6 ± 19.1 |
| 2s^22p^3(2P_3/2)_15l (l ≥ 2) | 18.139 | 18.282 | 18.134 | 35.1 | 47.4 | 40.1 |
| 2s^22p^3(2D_5/2)_37l (l ≥ 0) | 18.242 | 18.328 | 18.245 | 7.6 | 7.7 | 8.3 |
| 2s^22p^3(2D_5/2)_38l (l ≥ 0) | 18.429 | 18.510 | 18.431 | 7.0 | 7.1 | 7.6 |
| 2s^22p^3(2P_3/2)_19l (l ≥ 0) | 18.594 | 18.628 | 18.584 | 12.8 | 23.3 | 13.3 |
| 2s^22p^3(2D_5/2)_39l (l ≥ 0) | 18.601 | 18.678 | 18.603 | 6.4 | 6.5 | 6.9 |
| Blend | 18.307 | 18.419 | 18.297 | 18.255 ± 0.029 | 68.9 | 92.0 | 76.2 | 91.5 ± 12.1 |
| 2s^22p^3(2D_5/2)_nl (n = 40 – 44, l ≥ 0) | 19.017 | 19.084 | 19.018 | 18.968 ± 0.032 | 25.1 | 25.5 | 27.3 | 26.3 ± 10.2 |
| 2s^22p^3(2D_5/2)_nl (n = 45 – 53, l ≥ 0) | 19.737 | 19.783 | 19.732 | 27.7 | 28.1 | 30.1 |
| 2s^22p^3(2P_3/2)_nl (n = 45 – 53, l ≥ 0) | 19.930 | 19.939 | 19.921 | 10.3 | 18.0 | 10.5 |
| 2s^22p^3(2P_3/2)_nl (J = 0, 1) | 20.085 | 20.128 | 20.019 | 11.3 | 13.1 | 15.0 |
| Blend | 19.857 | 19.907 | 19.845 | 19.913 ± 0.027 | 49.3 | 59.2 | 55.6 | 47.1 ± 11.0 |
| 2s^22p^3(2D_5/2)_nl (n = 54 – 63, l ≥ 0) | 20.367 | 20.401 | 20.365 | 20.375 ± 0.021 | 17.5 | 17.7 | 19.0 | 19.1 ± 6.5 |
| 2s^22p^3(2P_3/2)_nl (l ≥ 0) | 20.781 | 20.906 | 20.759 | 27.6 | 51.3 | 33.8 |
| Dominant component | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) |
|--------------------|-----------|----------------------------|
| $2s^22p^3(2D_{5/2})nl$ \(n = 64 - 76, \ l \geq 0\) | 20.807 | 20.833 20.803 | 13.0 13.2 14.2 |
| $2s^22p^3(4P_{3/2})8s_{1/2}$ \(J = 2\) | 20.941 | 20.865 20.912 | 13.0 17.5 18.2 |
| Blend | 20.826 | 20.885 20.811 20.866 ± 0.022 | 53.6 82.0 66.2 61.1 ± 9.9 |
| $2s^22p^3(2P_{1/2})21l$ \(l \geq 0\) | 21.080 | 21.089 21.072 | 8.4 17.5 8.6 |
| $2s^22p^3(4P_{3/2})8s_{1/2}$ \(J = 1\) | 21.157 | 21.088 21.131 | 6.5 6.2 8.0 |
| $2s^22p^3(2D_{5/2})nl$ \(n = 77 - 120, \ l \geq 0\) | 21.247 | 21.260 21.243 | 16.8 17.0 18.4 |
| Blend | 21.184 | 21.160 21.175 21.203 ± 0.032 | 31.7 40.7 35.0 39.6 ± 7.8 |
| $2s^22p^3(2P_{1/2})22l$ \(l \geq 0\) | 22.076 | 22.083 22.069 | 4.8 10.6 4.8 |
| $2s^22p^3(4P_{3/2})8p_{1/2}$ \(J = 1\) | 22.296 | 22.237 22.285 | 15.3 14.7 15.3 |
| $2s^22p^3(4P_{3/2})8p_{1/2}$ \(J = 2\) | 22.448 | 22.394 22.438 | 27.3 26.5 27.4 |
| $2s^22p^3(4P_{3/2})8p_{3/2}$ \(J = 3\) | 22.448 | 22.403 22.449 | 31.9 31.0 31.8 |
| Blend | 22.396 | 22.330 22.390 22.413 ± 0.028 | 79.3 82.8 79.3 71.6 17.7 |
| $2s^22p^3(4P_{3/2})8p_{3/2}$ \(J = 2\) | 22.609 | 22.566 22.610 | 41.5 33.3 37.3 |
| $2s^22p^3(4P_{3/2})8p_{3/2}$ \(J = 1\) | 22.688 | 22.640 22.683 | 26.7 21.4 23.9 |
| $2s^22p^3(4P_{3/2})8p_{3/2}$ \(J = 0\) | 22.781 | 22.730 22.774 | 5.6 4.6 5.3 |
| $2s^22p^3(2P_{3/2})17l$ \(l \leq 1\) | 22.835 | 22.868 22.815 | 1.5 1.4 2.1 |
| Blend | 22.654 | 22.611 22.654 22.600 ± 0.022 | 75.3 60.7 68.6 80.0 ± 15.3 |
| $2s^22p^3(2P_{1/2})23l$ \(l \geq 0\) | 22.945 | 22.949 22.938 | 4.1 8.4 4.1 |
| $2s^22p^3(2D_{3/2})7s$ \(J = 1, 2\) | 22.824 | 23.043 22.949 | 1.9 2.0 2.8 |
| $2s^22p^3(2P_{3/2})17l$ \(l \geq 2\) | 23.017 | 23.114 23.004 | 10.6 13.9 13.0 |
| Blend | 22.977 | 23.051 23.983 23.097 ± 0.065 | 16.6 24.3 19.9 15.1 ± 13.8 |
| $2s^22p^3(2P_{1/2})6p_{1/2}$ \(J = 0\) | 23.461 | 23.516 23.410 | 0.00 0.01 0.01 |
| $2s^22p^3(2P_{1/2})6p_{1/2}$ \(J = 1\) | 23.571 | 23.644 23.529 | 2.7 2.6 2.4 |
| $2s^22p^3(2P_{1/2})6p_{3/2}$ \(J = 2\) | 23.681 | 23.781 23.671 | 0.4 0.4 0.4 |
| $2s^22p^3(2P_{1/2})8s$ \(J = 1\) | 23.678 | 23.673 23.680 | 7.7 9.2 10.7 |
| $2s^22p^3(2P_{1/2})24l$ \(l \geq 0\) | 23.708 | 23.696 23.706 | 3.5 6.3 3.4 |
| $2s^22p^3(4P_{3/2})8s_{3/2}$ \(J = 0\) | 23.849 | 23.786 23.834 | 6.2 4.2 3.3 |
| $2s^22p^3(2P_{1/2})6p_{3/2}$ \(J = 1\) | 23.900 | 23.988 23.878 | 10.0 10.0 8.5 |
| Blend | 23.780 | 23.826 23.747 23.752 ± 0.014 | 30.5 30.1 28.7 34.6 ± 10.1 |
Table 2—Continued

| Dominant component | $E_d$ (eV) | $S_d$ ($10^{-21}$ cm$^2$ eV) |
|--------------------|-----------|-----------------------------|
|                    | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
| $2s^2p^6(4s^2)5d_{3/2}$ ($J = 1$) | 23.904 | 23.855 | 23.906 | 20.9 | 18.1 | 20.0 |
| $2s^2p^6(4s^2)5d_{5/2}$ ($J = 4$) | 23.937 | 23.811 | 23.928 | 45.5 | 44.1 | 47.0 |
| $2s^2p^6(4s^2)5d_{5/2}$ ($J = 2$) | 23.985 | 23.935 | 23.984 | 34.7 | 30.7 | 33.8 |
| $2s^2p^6(4s^2)5d_{5/2}$ ($J = 3$) | 24.027 | 23.975 | 24.021 | 43.7 | 40.5 | 44.7 |
| Blend | 23.971 | 23.895 | 23.967 | 23.980 ± 0.007 | 144.8 | 133.4 | 145.5 | 144.1 ± 8.0 |
| $2s^2p^6(4s^2)5d_{3/2}$ ($J = 3$) | 24.229 | 24.179 | 24.223 | 62.6 | 46.1 | 55.8 |
| $2s^2p^6(4s^2)5d_{5/2}$ ($J = 2$) | 24.289 | 24.238 | 24.284 | 51.3 | 38.5 | 46.4 |
| $2s^2p^6(4s^2)5d_{5/2}$ ($J = 1$) | 24.359 | 24.308 | 24.354 | 44.8 | 31.7 | 39.4 |
| $2s^2p^6(4s^2)5d_{3/2}$ ($J = 2$) | 24.380 | 24.557 | 24.380 | 3.0 | 4.5 | 2.9 |
| Blend | 24.287 | 24.246 | 24.281 | 24.274 ± 0.080 | 161.7 | 120.8 | 144.5 | 132.7 ± 11.3 |
| $2s^2p^6(2D_{3/2})4f_{3/2}1^{18}f$ ($J = 0, 1, 2, 3$) | 24.846 | 24.935 | 24.831 | 9.5 | 12.1 | 11.5 |
| $2s^2p^6(4s^2)5f_{5/2}$ ($J = 1, 2$) | 24.951 | 24.886 | 24.933 | 806.2 | 846.1 | 858.0 |
| $2s^2p^6(4s^2)5f_{3/2}$ ($J = 0, 0, 1$) | 25.124 | 25.180 | 25.000 | 6.3 | 0.4 | 0.6 |
| $2s^2p^6(4s^2)5f_{3/2}$ ($J = 2$) | 25.028 | 25.118 | 25.097 | 1.0 | 1.3 | 1.5 |
| $2s^2p^6(4s^2)5f_{3/2}$ ($J = 1, 2$) | 25.228 | 25.111 | 25.267 | 18.5 | 18.4 | 19.3 |
| Blend | 24.961 | 24.901 | 24.943 | 24.978 ± 0.035 | 858.2 | 900.7 | 913.9 | 816.6 ± 137.6 |
| $2s^2p^6(2F_{3/2})5p_{1/2}$ ($J = 1, 2$) | 25.258 | 25.466 | 25.369 | 2.4 | 3.0 | 3.4 |
| $2s^2p^6(4s^2)5p_{3/2}$ ($J = 1$) | 25.416 | 25.438 | 25.410 | 25.3 | 19.7 | 22.6 |
| Blend | 25.402 | 25.442 | 25.405 | 25.583 ± 0.017 | 27.7 | 22.7 | 26.0 | 11.0 ± 5.9 |
| $2s^2p^6(2F_{3/2})5p_{1/2}$ ($J = 1, 2$) | 26.412 | 26.491 | 26.400 | 26.415 ± 0.075 | 7.6 | 9.6 | 9.1 | 21.6 ± 9.9 |
| $2s^2p^6(4s^2)5p_{3/2}$ ($J = 2$) | 26.695 | 26.710 | 26.688 | 28.1 | 26.2 | 28.9 |
| $2s^2p^6(4s^2)5p_{1/2}$ ($J = 1$) | 26.707 | 26.724 | 26.704 | 21.4 | 18.2 | 20.7 |
| $2s^2p^6(4s^2)5p_{3/2}$ ($J = 3$) | 26.752 | 26.764 | 26.740 | 50.1 | 44.2 | 49.4 |
| Blend | 26.726 | 26.740 | 26.717 | 26.742 ± 0.008 | 99.6 | 88.6 | 99.0 | 88.2 ± 6.5 |
| $2s^2p^6(5s^2)6d_{5/2}$ ($J = 2$) | 27.084 | 27.100 | 27.074 | 27.062 ± 0.014 | 55.3 | 39.7 | 48.4 | 23.8 ± 5.5 |
| $2s^2p^6(2D_{3/2})7d$ | 27.547 | 27.616 | 27.504 | 15.0 | 15.3 | 15.4 |
| $2s^2p^6(2D_{3/2})7d$ | 27.638 | 27.672 | 27.589 | 13.8 | 11.9 | 15.2 |


| Dominant component | $E_d$ (eV) | $S_d$ (10$^{-21}$ cm$^2$ eV) |
|--------------------|-----------|-----------------------------|
|                    | AUTOSTRUCTURE$^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
| 2s2p$^4$(4P$^0$/2)8l ($l \geq 3$) | 27.667 | 27.674 | 27.650 | 404.4 | 424.4 | 422.0 |
| 2s2p$^3$(3P$^3$/2)20l ($l \geq 0$) | 27.749 | 27.796 | 27.738 | 6.2 | 7.0 | 8.5 |
| Blend | 27.663 | 27.674 | 27.645 | 27.715 ± 0.006 | 439.4 | 458.6 | 461.1 | 424.9 ± 9.4 |
| 2s2p$^4$(2D$^5$/2)7l ($l \geq 3$) | 28.707 | 28.943 | 28.853 | 40.5 | 40.6 | 44.1 |
| 2s2p$^4$(2P$^2$/2)21l ($l \geq 0$) | 28.899 | 28.945 | 28.889 | 5.1 | 4.9 | 6.2 |
| 2s2p$^3$(2P$^1$/2)6f | 29.391 | 29.468 | 29.362 | 3.2 | 3.5 | 3.5 |
| Blend | 28.772 | 28.981 | 28.890 | 29.001 ± 0.044 | 48.8 | 49.0 | 53.8 | 59.6 ± 15.0 |
| 2s2p$^3$(2P$^1$/2)6l ($l = 4, 5$) | 29.666 | 29.748 | 29.644 | 1.9 | 2.1 | 1.5 |
| 2s2p$^4$(2D$^5$/2)7d | 29.612 | 29.766 | 29.702 | 0.8 | 0.6 | 0.5 |
| 2s2p$^4$(4P$^0$/2)9s | 29.861 | 29.879 | 29.789 | 11.5 | 13.9 | 15.7 |
| 2s2p$^3$(2P$^1$/2)22l ($l \geq 0$) | 29.895 | 29.939 | 29.886 | 4.3 | 4.1 | 5.2 |
| Blend | 29.838 | 29.874 | 29.801 | 29.918 ± 0.019 | 18.5 | 20.7 | 22.9 | 40.4 ± 7.2 |
| 2s2p$^4$(2P$^0$/2)23l ($l \geq 0$) | 30.765 | 30.807 | 30.756 | 3.7 | 3.3 | 4.4 |
| 2s2p$^4$(2D$^5$/2)7l ($l \geq 3$) | 30.800 | 30.849 | 30.765 | 0.8 | 0.7 | 0.7 |
| 2s2p$^4$(4P$^0$/2)9p | 30.992 | 31.033 | 30.970 | 91.9 | 83.7 | 89.7 |
| 2s2p$^3$(2P$^0$/2)24l ($l \geq 0$) | 31.527 | 31.553 | 31.519 | 3.2 | 2.5 | 3.8 |
| Blend | 30.999 | 31.038 | 30.980 | 31.038 ± 0.018 | 99.6 | 90.2 | 98.6 | 95.0 ± 13.4 |
| 2s2p$^4$(4P$^0$/2)9d$^5$/2 ($J = 4$) | 31.882 | 31.938 | 31.867 | 21.5 | 21.4 | 22.6 |
| 2s2p$^4$(4P$^0$/2)9d$^3$/2 ($J = 3$) | 31.881 | 31.939 | 31.870 | 17.7 | 18.0 | 18.8 |
| 2s2p$^4$(4P$^0$/2)9d$^2$/2 ($J = 2$) | 31.912 | 31.972 | 31.904 | 13.4 | 13.4 | 14.1 |
| 2s2p$^3$(2P$^0$/2)9d$^2$/2 ($J = 5$) | 31.912 | 32.009 | 31.937 | 29.7 | 29.3 | 31.3 |
| 2s2p$^3$(2P$^0$/2)9d$^2$/2 ($J = 1$) | 31.955 | 32.016 | 31.949 | 8.5 | 8.3 | 8.8 |
| Blend | 31.917 | 31.973 | 31.904 | 32.006 ± 0.010 | 90.8 | 90.4 | 95.6 | 78.3 ± 9.3 |
| 2s2p$^4$(4P$^0$/2)9d$^2$/2 ($J = 4$) | 32.091 | 32.150 | 32.076 | 16.2 | 12.9 | 15.4 |
| 2s2p$^3$(2P$^0$/2)25l ($l \geq 0$) | 32.200 | 32.412 | 32.192 | 2.7 | 2.2 | 3.3 |
| 2s2p$^3$(4P$^0$/2)9d$^2$/2 ($J = 0$) | 32.217 | 32.272 | 32.203 | 6.0 | 4.5 | 5.3 |
| 2s2p$^4$(4P$^0$/2)9d$^2$/2 ($J = 3$) | 32.247 | 32.304 | 32.232 | 36.2 | 23.9 | 29.7 |
| 2s2p$^4$(4P$^0$/2)9d$^2$/2 ($J = 1$) | 32.251 | 32.307 | 32.237 | 22.0 | 15.6 | 18.6 |
| 2s2p$^4$(4P$^0$/2)9d$^2$/2 ($J = 2$) | 32.279 | 32.337 | 32.266 | 38.7 | 27.0 | 32.5 |
| Blend | 32.235 | 32.293 | 32.218 | 32.376 ± 0.011 | 121.8 | 86.1 | 104.8 | 105.9 ± 11.6 |
| Dominant component | AUTOSTRUCTURE $^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
|-------------------|-------------------|-------------|-----------|-----------------|----------------|--------|------|--------------|
| $2s^2p^4(4P_{3/2})9l$ ($l \geq 3$) | 32.642 | 32.702 | 32.621 | 662.8 | 555.6 | 709.0 |
| $2s^2p^4(2P_{3/2})26l$ ($l \geq 0$) | 32.796 | 32.999 | 32.789 | 1.9 | 1.8 | 2.5 |
| Blend | 32.642 | 32.702 | 32.622 | 32.745 ± 0.002 | 664.7 | 557.4 | 711.5 | 621.0 ± 11.7 |
| $2s^2p^3(2P_{3/2})n l$ ($27 \leq n \leq 120$, $l \geq 0$) | 33.255-39.743 | 33.296-39.732 | 33.245-39.745 | 33.125 – 40.089 | 20.5 | 18.5 | 25.7 | 54.3 ± 46.6 |
| $2s^2p^4(4P_{3/2})9s$ ($J = 1, 2$) | 38.314 | 38.334 | 38.286 | 38.362 ± 0.091 | 6.5 | 7.6 | 8.6 | 14.4 ± 8.5 |
| $2s^2p^4(4P_{3/2})9p$ | 39.383 | 39.433 | 39.374 | 39.412 ± 0.016 | 59.3 | 53.5 | 56.5 | 43.2 ± 6.6 |
| $2s^2p^4(4P_{3/2})9d$ | 40.499 | 40.543 | 40.482 | 40.529 ± 0.011 | 116.7 | 100.3 | 115.0 | 98.7 ± 7.5 |
| $2s^2p^4(4P_{1/2})9s$ ($J = 1$) | 41.008 | 41.038 | 41.014 | 2.7 | 3.1 | 3.5 |
| $2s^2p^4(4P_{3/2})9l$ ($l \geq 3$) | 41.079 | 41.142 | 41.062 | 343.2 | 343.8 | 374.5 |
| Blend | 41.078 | 41.142 | 41.062 | 41.112 ± 0.003 | 345.9 | 346.9 | 378.0 | 325.5 ± 6.7 |
| $2s^2p^4(2S_{1/2})7s$ ($J = 0, 1$) | 42.023 | 42.073 | 41.974 | 1.0 | 1.2 | 1.4 |
| $2s^2p^4(4P_{1/2})9p$ | 42.115 | 42.163 | 42.100 | 25.1 | 23.5 | 24.9 |
| $2s^2p^4(4P_{3/2})10s$ ($J = 2, 3$) | 42.154 | 42.155 | 42.127 | 6.1 | 7.3 | 8.1 |
| Blend | 42.120 | 42.158 | 42.101 | 42.112 ± 0.041 | 32.2 | 32.0 | 34.4 | 94.8 ± 13.3 |
| $2s^2p^4(4P_{3/2})10p$ | 42.976 | 42.993 | 42.955 | 47.9 | 44.2 | 47.1 |
| $2s^2p^4(4P_{3/2})9d_{3/2}$ ($J = 2$) | 43.109 | 43.169 | 43.100 | 11.4 | 10.9 | 11.9 |
| $2s^2p^4(4P_{3/2})9d_{5/2}$ ($J = 1$) | 43.117 | 43.179 | 43.111 | 8.5 | 7.5 | 8.3 |
| $2s^2p^4(4P_{3/2})9d_{5/2}$ ($J = 3$) | 43.149 | 43.207 | 43.136 | 19.6 | 18.0 | 19.7 |
| Blend | 43.046 | 43.082 | 43.031 | 43.104 ± 0.011 | 87.4 | 80.6 | 87.0 | 74.3 ± 6.3 |
| $2s^2p^4(4P_{3/2})9d_{5/2}$ ($J = 2$) | 43.381 | 43.441 | 43.369 | 18.7 | 13.6 | 16.4 |
| $2s^2p^4(4P_{3/2})10d$ | 43.776 | 43.784 | 43.747 | 110.3 | 94.0 | 104.0 |
| $2s^2p^4(4P_{3/2})9l$ ($l \geq 3$) | 43.795 | 43.865 | 43.779 | 180.4 | 180.1 | 190.0 |
| Blend | 43.763 | 43.818 | 43.747 | 43.831 ± 0.006 | 309.4 | 287.7 | 310.4 | 303.7 ± 10.4 |
| $2s^2p^4(4P_{3/2})10l$ ($l \geq 3$) | 44.176 | 44.208 | 44.152 | 44.241 ± 0.003 | 364.3 | 303.5 | 394.0 | 333.0 ± 9.0 |
| $2s^2p^4(2S_{1/2})7d$ | 46.525 | 46.594 | 46.505 | 46.526 ± 0.020 | 3.2 | 2.9 | 3.5 | 9.9 ± 2.4 |
| $2s^2p^4(2P_{3/2})7s$ ($J = 1, 2$) | 47.796 | 47.840 | 47.748 | 3.6 | 4.4 | 5.1 |
| $2s^2p^4(2S_{1/2})7l$ ($l \geq 3$) | 47.847 | 47.923 | 47.791 | 5.1 | 7.0 | 7.2 |
| Dominant component | AUTOSTRUCTURE $^a$ | HULLAC$^a$ | MCDF$^a$ | Experiment$^{b,c}$ | AUTOSTRUCTURE | HULLAC | MCDF | Experiment$^b$ |
|--------------------|--------------------|-------------|-----------|----------------------|--------------|--------|------|----------------|
| Blend              | 47.826             | 47.891      | 47.777    | 47.865 ± 0.093       | 8.7          | 11.4   | 12.3 | 17.8 ± 4.8    |
| 2s2p$^4(2p_{3/2})7p_{3/2}$ ($J = 1$) | 50.452             | 50.541      | 50.444    | 1.8                  | 2.2          | 2.0    |      |                |
| 2s2p$^4(4p_{3/2})10s$ ($J = 1, 2$) | 50.603             | 50.605      | 50.579    | 3.3                  | 3.9          | 4.3    |      |                |
| Blend              | 50.550             | 50.582      | 50.536    | 50.634 ± 0.079       | 5.1          | 6.1    | 6.3  | 6.3 ± 3.4     |
| 2s2p$^4(4p_{5/2})11s$ ($J = 2, 3$) | 51.194             | 51.180      | 51.169    | 4.0                  | 4.8          | 5.3    |      |                |
| 2s2p$^4(4p_{5/2})10p$ | 51.362             | 51.406      | 51.372    | 31.8                 | 29.0         | 30.6   |      |                |
| 2s2p$^4(2d_{3/2})8d_{3/2}$ ($J = 3$) | 51.520             | 51.522      | 51.415    | 1.5                  | 1.1          | 1.2    |      |                |
| Blend              | 51.367             | 51.379      | 51.344    | 51.346 ± 0.023       | 37.3         | 34.9   | 37.1 | 45.5 ± 4.8    |
| 2s2p$^4(4p_{5/2})11p$ | 51.809             | 51.806      | 51.789    | 51.852 ± 0.050       | 30.7         | 28.6   | 30.3 | 36.2 ± 4.5    |
| 2s2p$^4(2d_{3/2})8l$ ($l \geq 3$) | 52.258             | 52.509      | 52.402    | 12.6                 | 12.8         | 14.2   |      |                |
| 2s2p$^4(4p_{3/2})10l$ ($l \geq 2$) | 52.514             | 52.562      | 52.507    | 285.3                | 283.5        | 303.0  |      |                |
| 2s2p$^4(4p_{5/2})11l$ ($l \geq 2$) | 52.643             | 52.651      | 52.622    | 319.3                | 282.6        | 308.0  |      |                |
| 2s2p$^4(2p_{3/2})7d$ | 52.517             | 52.556      | 52.746    | 10.4                 | 9.9          | 11.4   |      |                |
| Blend              | 52.575             | 52.603      | 52.565    | 52.640 ± 0.016       | 627.6        | 588.8  | 636.6| 533.0 ± 7.3  |
| 2s2p$^4(2p_{3/2})7l$ ($l \geq 3$) | 53.695             | 53.773      | 53.678    | 17.5                 | 24.7         | 25.0   |      |                |
| 2s2p$^4(4p_{3/2})11l$ ($l \leq 1$) | 54.107             | 54.031      | 53.991    | 14.7                 | 15.9         | 16.7   |      |                |
| Blend              | 53.883             | 53.874      | 53.803    | 53.982 ± 0.056       | 32.2         | 40.6   | 41.7 | 47.1 ± 9.5    |
| 2s2p$^4(4p_{1/2})10d$ | 54.901             | 54.923      | 54.883    | 54.876 ± 0.033       | 33.7         | 29.7   | 32.8 | 20.8 ± 5.9    |
| 2s2p$^4(4p_{1/2})10l$ ($l \geq 3$) | 55.331             | 55.374      | 55.316    | 55.320 ± 0.007       | 118.0        | 122.9  | 126.0| 147.4 ± 7.3  |
| 2s2p$^4(4p_{1/2})12p$ | 58.506             | 58.487      | 58.486    | 58.498 ± 0.065       | 21.6         | 20.3   | 21.5 | 35.8 ± 9.6    |
| 2s2p$^4(4p_{5/2})12l$ ($l \geq 2$) | 59.151             | 59.142      | 59.132    | 59.210 ± 0.004       | 239.4        | 211.5  | 235.0| 204.2 ± 6.1  |
| 2s2p$^4(4p_{3/2})11p$ | 60.223             | 60.226      | 60.212    | 60.2 − 60.5$^c$      | 21.2         | 19.5   | 20.5 | 9.0 ± 5.0     |
| 2s2p$^4(4p_{3/2})11d$ | 60.825             | 60.826      | 60.811    | 60.784 ± 0.040       | 44.4         | 39.3   | 43.3 | 49.1 ± 11.9   |
| 2s2p$^4(4p_{3/2})11l$ ($l \geq 3$) | 61.149             | 61.162      | 61.134    | 61.152 ± 0.009       | 162.2        | 162.9  | 177.0| 148.7 ± 11.4 |
| 2s2p$^4(4p_{1/2})11p$ | 62.946             | 62.949      | 62.931    | 62.940 ± 0.059       | 9.9          | 9.5    | 9.9  | 17.3 ± 5.1    |
| 2s2p$^4(4p_{3/2})13s$ ($J = 2, 3$) | 63.334             | 63.295      | 63.303    | 2.3                  | 2.7          | 2.9    |      |                |
| 2s2p$^4(4p_{1/2})11d$ | 63.589             | 63.542      | 63.522    | 22.3                 | 20.0         | 21.8   |      |                |
| 2s2p$^4(4p_{3/2})10p$ | 63.704             | 63.672      | 63.684    | 16.3                 | 15.3         | 16.2   |      |                |
| Dominant component | \(E_d\) (eV) | \(S_d\) \(\times 10^{-21} \text{ cm}^2 \text{ eV}\) |
|--------------------|----------|----------------|
| Blend              | 63.620   | 63.921 ± 0.012 | 40.9  | 38.0  | 40.9  | 26.0 ± 4.9 |
| \(2s^2p^4(4P_{3/2})11f\) \((l \geq 3)\) | 63.866   | 64.228 ± 0.005 | 89.4  | 90.4  | 96.2  | \text{N/A} |
| \(2s^2p^4(4P_{5/2})13d\) | 64.063   | 64.306 ± 0.005 | 24.5  | 32.4  | 35.2  | \text{N/A} |
| Blend              | 63.908   | 67.184 ± 0.215 | 113.9 | 122.8 | 131.4 | 112.4 ± 5.6 |
| \(2s^2p^4(4P_{3/2})13f\) \((l \geq 3)\) | 64.250   | 64.634 ± 0.013 | 155.5 | 136.7 | 156.0 | 164.6 ± 3.9 |
| \(2s^2p^4(4P_{5/2})12f\) \((l \leq 2)\) | 67.236   | 67.624 ± 0.013 | 47.1  | 44.6  | 48.2  | 42.0 ± 32.1 |
| Blend              | 67.653   | 67.643 ± 0.013 | 145.5 | 142.7 | 158.2 | 142.6 ± 28.7 |
| \(2s^2p^4(4P_{3/2})14f\) \((l \geq 2)\) | 68.230   | 68.634 ± 0.013 | 169.7 | 151.5 | 173.4 | 156.4 ± 5.6 |
| Blend              | 68.237   | 68.224 ± 0.013 | 7.3   | 7.0   | 7.3   | 15.6 ± 5.6  |
| \(2s^2p^4(4P_{3/2})12p\) | 69.646   | 69.633 ± 0.013 | 7.3   | 7.0   | 7.3   | 15.6 ± 5.6  |
| \(2s^2p^4(4P_{3/2})12f\) \((l \geq 2)\) | 70.310   | 70.298 ± 0.010 | 89.6  | 87.0  | 94.7  | \text{N/A} |
| \(2s^2p^4(2S_{1/2})8d\) | 70.490   | 70.469 ± 0.010 | 81.5  | 88.5  | 96.4  | 90.0 ± 4.7  |
| Blend              | 70.313   | 70.301 ± 0.010 | \text{N/A} | \text{N/A} | \text{N/A} | \text{N/A} |
| \(2s^2p^4(2S_{1/2})8l\) \((l \geq 3)\) | 71.383   | 71.356 ± 0.010 | 2.9   | 3.6   | 3.5   | \text{N/A} |
| \(2s^2p^4(4P_{5/2})15f\) \((l \geq 0)\) | 71.442   | 71.419 ± 0.010 | 150.7 | 133.1 | 154.0 | \text{N/A} |
| \(2s^2p^4(4P_{3/2})13s\) \((J = 1, 2)\) | 71.778   | 71.750 ± 0.010 | 1.4   | 1.6   | 1.7   | \text{N/A} |
| Blend              | 71.444   | 71.421 ± 0.010 | 155.0 | 138.3 | 158.3 | 155.0 ± 4.8 |
| \(2s^2p^4(4P_{3/2})13p\) | 72.127   | 72.115 ± 0.005 | 11.8  | 11.0  | 11.5  | 16.6 ± 3.8  |
| \(2s^2p^4(4P_{3/2})13l\) \((l \geq 2)\) | 72.654   | 72.641 ± 0.005 | 72.73 ± 0.055 | 11.8 | 11.0 | 11.5 | 16.6 ± 3.8 |
| \(2s^2p^4(4P_{3/2})16f\) \((l \geq 0)\) | 74.098   | 74.172 ± 0.009 | 133.8 | 129.5 | 145.0 | 137.4 ± 4.6 |
| \(2s^2p^4(4P_{3/2})13p\) | 74.847   | 74.880 ± 0.012 | 7.3   | 7.3   | 7.5   | 6.0 ± 4.1  |
| \(2s^2p^4(2P_{3/2})8p\) | 74.897   | 74.880 ± 0.012 | 5.6   | 5.4   | 5.6   | \text{N/A} |
| Blend              | 74.859   | 74.845 ± 0.012 | 1.7   | 1.9   | 1.9   | \text{N/A} |
Table 2—Continued

| Dominant component | AUTOSTRUCTURE a | HULLAC a | MCDF a | Experiment b,c | AUTOSTRUCTURE | HULLAC | MCDF | Experiment b |
|--------------------|----------------|----------|--------|----------------|--------------|---------|-------|---------------|
| 2s2p^4(4P_{3/2})13f (l ≥ 2) | 75.373 | 75.356 | 75.360 | 75.420 ± 0.013 | 75.2 | 72.0 | 79.8 | 72.0 ± 5.4 |
| 2s2p^4(4P_{3/2})17l (l ≥ 0) | 76.298 | 76.221 | 76.276 | | 116.8 | 117.6 | 123.0 | |
| 2s2p^4(2P_{3/2})8d | 76.424 | 76.498 | 76.392 | 5.3 | 5.3 | 5.9 | |
| 2s2p^4(4P_{3/2})14l (l ≤ 2) | 76.419 | 76.371 | 76.403 | 29.7 | 27.4 | 29.5 | |
| Blend | 76.326 | 76.258 | 76.304 | 76.332 ± 0.009 | 151.8 | 150.3 | 158.4 | 115.2 ± 5.5 |
| 2s2p^4(4P_{3/2})14l (l ≥ 3) | 76.696 | 76.662 | 76.680 | 76.727 ± 0.011 | 98.8 | 94.7 | 107.0 | 127.2 ± 5.5 |
| 2s2p^4(2P_{3/2})10l (l ≥ 3) | 77.233 | 77.320 | 77.209 | 77.278 ± 0.044 | 11.3 | 14.4 | 15.1 | 12.4 ± 3.9 |
| 2s2p^4(4P_{3/2})18l (l ≥ 0) | 78.140 | 78.055 | 78.119 | 78.218 ± 0.009 | 106.5 | 94.0 | 113.0 | 102.2 ± 5.4 |
| 2s2p^4(4P_{3/2})14l (l ≥ 0) | 79.361 | 79.321 | 79.342 | 79.448 ± 0.056 | 70.3 | 67.4 | 74.9 | 64.7 ± 22.2 |
| 2s2p^4(4P_{3/2})19l (l ≥ 0) | 79.690 | 79.612 | 79.678 | | 98.4 | 96.5 | 109.0 | |
| 2s2p^4(2D_{5/2})10l (l ≥ 0) | 79.841 | 79.925 | 79.861 | 7.3 | 8.0 | 9.1 | |
| 2s2p^4(4P_{3/2})15l (l ≥ 0) | 79.888 | 79.835 | 79.866 | 111.9 | 107.4 | 120.0 | |
| Blend | 79.801 | 79.737 | 79.782 | 79.866 ± 0.023 | 217.6 | 211.9 | 233.1 | 197.0 ± 23.1 |
| 2s2p^4(4P_{3/2})20l (l ≥ 0) | 81.029 | 80.924 | 81.008 | 81.090 ± 0.008 | 91.7 | 87.7 | 97.4 | 92.0 ± 5.3 |
| 2s2p^4(4P_{3/2})21l (l ≥ 0) | 82.174 | 82.055 | 82.153 | 82.202 ± 0.022 | 86.0 | 76.1 | 91.4 | 86.9 ± 16.1 |
| 2s2p^4(4P_{3/2})16l (l ≥ 1) | 82.544 | 82.483 | 82.522 | | 100.7 | 104.3 | 109.0 | |
| 2s2p^4(4P_{3/2})15l (l ≥ 1) | 82.607 | 82.558 | 82.592 | 62.7 | 59.7 | 66.0 | |
| Blend | 82.568 | 82.510 | 82.548 | 82.578 ± 0.019 | 163.4 | 164.0 | 175.0 | 148.7 ± 16.2 |
| 2s2p^4(4P_{3/2})22l (l ≥ 0) | 83.166 | 83.054 | 83.145 | 83.225 ± 0.012 | 81.1 | 74.5 | 86.3 | 87.2 ± 6.7 |
| 2s2p^4(4P_{3/2})n\ell (23 ≥ n ≤ 120, l ≥ 0) | 84.031-92.986 | 83.775-92.990 | 83.854-92.966 | 2371.6 | 1823.5 | 2487.4 | |
| 2s2p^4(4P_{3/2})n\ell (17 ≥ n ≤ 120, l ≥ 0) | 84.740-101.425 | 84.580-101.431 | 84.337-101.408 | 2337.2 | 1929.4 | 2419.5 | |
| 2s2p^4(4P_{1/2})n\ell (16 ≥ n ≤ 120, l ≥ 0) | 85.257-104.140 | 84.734-104.149 | 84.782-104.125 | 1339.8 | 1161.1 | 1396.1 | |
| Blend | 84.031-104.140 | 83.775-104.149 | 83.854-104.125 | 83.600 – 104.485 | 6048.6 | 4914.0 | 6303.0 | 5250.8 ± 55.5 |
| 2s2p^4(2P_{3/2})10l (l ≥ 2) | 104.80 | 104.85 | 104.78 | 10.3 | 10.9 | 12.7 | |
| 2s2p^4(2P_{1/2})9l (l ≥ 2) | 105.01 | 105.09 | 104.99 | 0.5 | 0.5 | 0.5 | |
| Blend | 104.81 | 104.86 | 104.79 | 104.98 ± 0.04 | 10.8 | 11.4 | 13.2 | 22.5 ± 5.4 |
| Dominant component | AUTOSTRUCTURE | HULLAC<sup>a</sup> | MCDF<sup>a</sup> | Experiment<sup>b,c</sup> |
|--------------------|---------------|----------------|---------------|------------------------|
|                    | AUTOSTRUCTURE | HULLAC | MCDF | Experiment<sup>b</sup> |

<sup>a</sup>Weighted energy: \( E_d = \sum E_d S_d / \sum S_d \).

<sup>b</sup>1σ statistical fitting uncertainties only.

<sup>c</sup>Absolute energy scale uncertainty \( \lesssim 0.5\% \) for \( E \lesssim 25 \text{ eV} \) and \( \lesssim 0.2\% \) for \( E \gtrsim 25 \text{ eV} \).

<sup>d</sup>See § 3 about the experimental results.

<sup>e</sup>See § 5 about the theoretical results.

<sup>f</sup>Unable to fit for resonance energy.
Table 3. Rate coefficient fit parameters for $\Delta N = 0$ DR of Fe XX forming Fe XIX ($n_{\text{max}} = 120$). The units are $\text{cm}^3 \text{s}^{-1} \text{K}^{1.5}$ for $c_i$ and eV for $E_i$.

| Parameter | Experiment | AUTOSTRUCTURE | HULLAC | MCDF | R-matrix |
|-----------|------------|---------------|--------|------|----------|
| $c_1$     | 8.53E-05   | 1.38E-05      | 6.25E-05 | 4.51E-06 | 9.80E-06 |
| $c_2$     | 1.62E-04   | 3.29E-05      | 9.68E-05 | 2.88E-06 | 3.47E-05 |
| $c_3$     | 7.71E-05   | 3.02E-06      | 2.69E-04 | 1.41E-04 | 3.25E-05 |
| $c_4$     | 4.04E-05   | 1.96E-04      | 3.19E-04 | 8.29E-05 | 3.04E-05 |
| $c_5$     | 1.75E-04   | 5.17E-04      | 3.08E-03 | 1.84E-04 | 1.35E-04 |
| $c_6$     | 6.73E-04   | 2.49E-03      | 3.01E-03 | 5.45E-04 | 1.30E-04 |
| $c_7$     | 2.85E-03   | 2.92E-03      | 7.62E-03 | 3.37E-03 | 6.57E-04 |
| $c_8$     | 3.18E-03   | 2.13E-03      | 1.55E-02 | 3.98E-03 | 3.06E-03 |
| $c_9$     | 1.40E-02   | 9.27E-03      | 5.97E-02 | 1.75E-02 | 3.60E-03 |
| $c_{10}$  | 2.88E-03   | 9.40E-03      | 2.33E-03 | 7.44E-02 | 1.47E-02 |
| $c_{11}$  | 5.78E-02   | 7.55E-02      | ...     | 9.05E-03 | 9.41E-03 |
| $c_{12}$  | 1.26E-02   | ...           | ...     | ...     | 5.26E-02 |
| $c_{13}$  | ...        | ...           | ...     | ...     | 1.30E-02 |
| $E_1$     | 1.07E-03   | 1.02E-03      | 6.34E-02 | 4.04E-04 | 5.83E-04 |
| $E_2$     | 4.42E-03   | 3.59E-03      | 1.01E-01 | 1.44E-03 | 3.19E-03 |
| $E_3$     | 1.34E-02   | 1.40E-02      | 2.91E-01 | 4.57E-02 | 7.34E-03 |
| $E_4$     | 5.00E-02   | 6.46E-02      | 5.00E-01 | 9.37E-02 | 2.71E-02 |
| $E_5$     | 1.29E-01   | 2.99E-01      | 1.37E+00 | 2.49E-01 | 5.45E-02 |
| $E_6$     | 3.57E-01   | 1.14E+00      | 3.67E+00 | 4.71E-01 | 1.26E-01 |
| $E_7$     | 1.30E+00   | 2.86E+00      | 1.11E+01 | 1.45E+00 | 4.02E-01 |
| $E_8$     | 3.29E+00   | 4.98E+00      | 2.76E+01 | 4.23E+00 | 1.35E+00 |
Table 3—Continued

| Parameter | Experiment | AUTOSTRUCTURE | HULLAC  | MCDF   | R-matrix |
|-----------|------------|---------------|---------|--------|----------|
| E₉        | 1.33E+01   | 1.42E+01      | 8.52E+01| 1.60E+01| 3.69E+00 |
| E₁₀       | 3.76E+01   | 2.04E+01      | 2.52E+02| 7.40E+01| 1.46E+01 |
| E₁₁       | 6.60E+01   | 7.98E+01      | ...     | 2.29E+02| 4.63E+01 |
| E₁₂       | 2.12E+02   | ...           | ...     | ...    | 7.21E+01 |
| E₁₃       | ...        | ...           | ...     | ...    | 1.50E+02 |
Table 4. R-matrix rate coefficient for RR of Fe XX forming Fe XIX as a function of plasma temperature for $n_{max} = \infty$. The R-matrix results have been topped-up using AUTOSTRUCTURE for RR into $J \geq 26$ levels.

| $k_B T_e$ (eV) | Rate ($k_B T_e$) (cm$^3$ s$^{-1}$) | Rate ($k_B T_e$) (cm$^3$ s$^{-1}$) | Rate ($k_B T_e$) (cm$^3$ s$^{-1}$) | Rate ($k_B T_e$) (cm$^3$ s$^{-1}$) |
|--------------|----------------|----------------|----------------|----------------|
| 0.001        | 1.347E-08      | 0.1            | 1.082E-09      | 10             |
|              |                |                | 6.071E-11      | 1000           |
| 0.002        | 9.578E-09      | 0.2            | 7.277E-10      | 20             |
|              |                |                | 3.832E-11      | 2000           |
| 0.003        | 7.759E-09      | 0.3            | 5.706E-10      | 30             |
|              |                |                | 2.896E-11      | 3000           |
| 0.004        | 6.639E-09      | 0.4            | 4.777E-10      | 40             |
|              |                |                | 2.353E-11      | 4000           |
| 0.005        | 5.871E-09      | 0.5            | 4.154E-10      | 50             |
|              |                |                | 1.995E-11      | 5000           |
| 0.006        | 5.309E-09      | 0.6            | 3.699E-10      | 60             |
|              |                |                | 1.740E-11      | 6000           |
| 0.007        | 4.875E-09      | 0.7            | 3.354E-10      | 70             |
|              |                |                | 1.549E-11      | 7000           |
| 0.008        | 4.530E-09      | 0.8            | 3.082E-10      | 80             |
|              |                |                | 1.400E-11      | 8000           |
| 0.009        | 4.249E-09      | 0.9            | 2.862E-10      | 90             |
|              |                |                | 1.280E-11      | 9000           |
| 0.01         | 4.014E-09      | 1              | 2.681E-10      | 100            |
|              |                |                | 1.182E-11      | 10000          |
| 0.02         | 2.769E-09      | 2              | 1.763E-10      | 200            |
|              |                |                | 6.953E-12      |                 |
| 0.03         | 2.203E-09      | 3              | 1.364E-10      | 300            |
|              |                |                | 5.020E-12      |                 |
| 0.04         | 1.861E-09      | 4              | 1.128E-10      | 400            |
|              |                |                | 3.942E-12      |                 |
| 0.05         | 1.628E-09      | 5              | 9.706E-11      | 500            |
|              |                |                | 3.249E-12      |                 |
| 0.06         | 1.460E-09      | 6              | 8.576E-11      | 600            |
|              |                |                | 2.764E-12      |                 |
| 0.07         | 1.332E-09      | 7              | 7.724E-11      | 700            |
|              |                |                | 2.405E-12      |                 |
| 0.08         | 1.231E-09      | 8              | 7.055E-11      | 800            |
|              |                |                | 2.129E-12      |                 |
| 0.09         | 1.150E-09      | 9              | 6.516E-11      | 900            |
|              |                |                | 1.909E-12      |                 |
Fig. 1.— Fe XX to Fe XIX $\Delta N = 0$ DR resonance structure: (a) Experimental, (b) AUTOSTRUCTURE, (c) HULLAC, (d) MCDF, and (e) R-matrix results. The experimental and theoretical data represent the DR and RR cross sections times the electron-ion relative velocity convolved with the energy spread of the experiment (i.e., a rate coefficient) and are shown versus electron-ion center-of-mass collision energy. In (a) resonances resulting from the $^4S_{3/2} - ^4P_{3/2}$, $^4S_{3/2} - ^4P_{3/2}$, and $^4S_{3/2} - ^4P_{1/2}$ core excitations are labeled for capture into high $l$ levels. Unlabeled resonances are due to capture into low $l$ levels or due to DR via other core excitations. Many of the unlabeled resonances below $\approx 40$ eV are due to DR via $2p_{1/2} - 2p_{3/2}$ core excitations. The nonresonant “background” rate coefficient in (a) is due primarily to RR. In (b), (c), and (d) we have added the convolved, non-resonant RR contribution obtained from our R-matrix calculations to our DR results.
Fig. 1.— Continued
Fig. 1.— Continued
Fig. 2.— Measured and fitted Fe XX to Fe XIX $\Delta N = 0$ DR resonance structure below 0.1 eV. The experimental results are shown by the solid curve. The dotted-long-dashed curve is the fit to the data using our calculated RR rate coefficient and taking into account all resolved resonances. The dotted curve is the fit including the estimated contributions from the unresolved $2s^2 2p^3 (^2D_{5/2}) 15l$ (short-dashed curves) and $2s2p^4 (^4P_{3/2}) 7d$ (long dashed curve) resonances (see § 3).
Fig. 3.— Fe XX to Fe XIX Maxwellian-averaged rate coefficient for $\Delta N = 0$ DR from $k_B T_e = 0.1$ to 300 eV. (a) The thick solid curve represents our experimentally-derived rate coefficient using the results shown in Figure 1(a) and listed in Table 2. The error bars represent the estimated maximum experimental uncertainty of 20% for $k_BT_e \geq 10$ eV. The long-dashed curve shows the $LS$-coupling calculations of Jacobs et al. (1977) as fitted by Shull & van Steenberg (1982). The short-dashed curve shows the unpublished $LS$-coupling calculations of Roszman as given by Arnaud & Raymond (1992). The thin solid curve is our R-matrix RR rate coefficient ($n_{\text{max}} = \infty$) which has been topped up using AUTOSTRUCTURE. Also shown is the recommended RR rate coefficient of Arnaud & Raymond (1992; dotted curve).
(b) In addition to our experimentally-derived DR rate coefficient (thick solid curve) and our topped up R-matrix RR rate coefficient (thin solid curve), both from (a), we also show our AUTOSTRUCTURE (short-dashed curve), HULLAC (dotted-long-dashed curve), MCDF (dotted curve), and R-matrix results (minus the R-matrix RR contribution, long dashed curve). All DR rate coefficients in (b) are for an $n_{\text{max}} = 120$. The formation zone for Fe XX for an optically thin, low-density photoionized plasma of cosmic abundances as predicted by XSTAR (Kallman & Bautista 2001) is shown by the horizontal solid line in both (a) and (b).
Fig. 4.— The ratio of the (a) AUTOSTRUCTURE, (b) HULLAC, and (c) MCDF resonance energies relative to the measured resonance energies as a function of center-of-mass collision energy from 0.07 to 100 eV.
Fig. 4.— Continued
Fig. 5.— Theoretical Fe XX to Fe XIX $\Delta N = 0$ DR resonance structure between 0.015 and 0.8 eV compared to our experimental results: (a) AUTOSTRUCTURE, (b) HULLAC, (c) MCDF, and (d) R-matrix results. See Figure 1 for details.
Fig. 5.— Continued
Fig. 5—Continued

Rate coefficient (10^{-10} \text{ cm}^3 \text{s}^{-1})

- Experiment (d)
- R-matrix
Fig. 6.— The ratio of the resonance strengths given in Table 2 for our (a) AUTOSTRUCTURE/experiment, (b) HULLAC/experiment, and (c) MCDF/experiment, results. Resonance strength ratios are shown as a function of center-of-mass collision energy from 0.07 to 100 eV. The solid lines show the average value for the various ratios. The dashed lines show the $1\sigma$ standard deviation from these average values.
Fig. 6.— Continued
Fig. 7.— The ratio of the resonance strengths given in Table 2 for our (a) AUTOSTRUCTURE/MCDF, (b) HULLAC/MCDF, and (c) HULLAC/AUTOSTRUCTURE results. Resonance strength ratios are shown as a function of center-of-mass collision energy from 0.07 to 100 eV. The solid lines show the average value for the various ratios. The dashed lines show the 1σ standard deviation from these average values.
Fig. 7.— Continued