K-shell photoabsorption cross sections for the isonuclear C\textsubscript{i}→C\textsubscript{iV} ions have been computed using the \textit{R}-matrix method. Above the K-shell threshold, the present results are in good agreement with the independent-particle results of Reilman & Manson. Below threshold, we also compute the strong 1\textit{s}→\textit{np} absorption resonances with the inclusion of important spectator Auger broadening effects. For the lowest 1\textit{s}→2\textit{p}, 3\textit{p} resonances, comparisons to available C\textsubscript{II}, C\textsubscript{III}, and C\textsubscript{IV} experimental results show good agreement in general for the resonance strengths and positions. Our results also provide detailed information on the C\textsubscript{i} K-shell photoabsorption cross section including the strong resonance features, since very limited laboratory experimental data exist. The resultant \textit{R}-matrix cross sections are then used to model the \textit{Chandra} X-ray absorption spectrum of the blazar Mkn 421.

\textit{Key words:} atomic data – atomic processes – BL Lacertae objects: individual (Mkn 421) – galaxies: active – ISM: lines and bands – X-rays: galaxies

\textit{Online-only material:} color figures

1. INTRODUCTION

The inner-shell excitation and ionization features of cosmically abundant elements fall in the spectral ranges covered by the high-resolution X-ray spectrometers on board the \textit{Chandra} and \textit{XMM-Newton} observatories. The detailed structure and wavelengths of absorption resonances of a given element depend on its ionization and chemical state. High-resolution X-ray spectroscopy of these features can in principle be used to probe the physics and chemistry of astrophysical plasmas. Inner-shell photoabsorption resonances have proven particularly useful for investigating the chemical composition of the interstellar gas in the line of sight toward bright sources of X-ray continuum radiation, as demonstrated in the pioneering study of Schattenburg & Canizares (1986; see also Paerels et al. 2001; Takei et al. 2002; de Vries et al. 2003; Juett et al. 2004, 2006; Ueda et al. 2005; Yao & Wang 2006; Yao et al. 2009; Kaastra et al. 2009). Ness et al. (2007) were able to identify several ionization stages of oxygen in the post-outburst circumstellar material of the recurrent nova RS Oph based on the prominent 1\textit{s}→2\textit{p} resonance.

These studies have all employed oxygen and higher Z elements. Carbon is the fourth most abundant element in the Galaxy (after H, He, and O), but has not yet been exploited as an X-ray photoabsorption diagnostic. It presents a special challenge for X-ray transmission spectroscopy. X-ray instruments often employ visible/UV light blocking filters based on carbon compounds that are robust to space deployment. These filters imprint strong C K-edge absorption signatures on X-ray spectra, rendering difficult the disentanglement of weaker astrophysical absorption features. The task is hampered further still by a current lack of data describing the expected absorption edge structure and resonances for neutral and ionized C.

To our knowledge, the only available data for carbon-ion K-shell photoabsorption data are the following. Theoretically, there are photoionization cross sections for all carbon ions that have been computed using the independent-particle (IP) model (Reilman & Manson 1979; Yeh 1993) or the scaled hydrogenic approximation (Verner et al. 1993; Verner & Yakovlev 1995). \textit{R}-matrix calculations have also been performed for C\textsubscript{i} above the K-shell threshold in order to investigate shake up and shake off processes, i.e., photoionization of the 1\textit{s} electron followed by excitation or ionization of a 2\textit{p} electron (Petri\`{n}i & da Silva 1999; McLaughlin 2001). While all of these calculations are quite reliable, only the \textit{R}-matrix calculations for neutral C (McLaughlin 2001) have included the strong 1\textit{s}→\textit{np} absorption features that form a Rydberg series of resonances below the K-shell threshold, giving a resonant photoabsorption cross section below threshold that matches smoothly to the above-threshold photoionization. All other theoretical work, for all other ions, only considered 1\textit{s}→\textit{np} photoionization above the K-shell threshold and did not include the 1\textit{s}→\textit{np} resonances. Experimentally, there exists cross section data from the work of Jannitti et al. (1990) and Nicolosi et al. (1991) primarily obtained from the dual laser plasma technique, as pioneered by Carroll & Kennedy (1977). There is also the cross section data obtained from carbon in its solid state by Henke and co-workers (Henke et al. 1982, 1993). The dual plasma technique is useful for obtaining absorption spectra over a wide energy range (Jannitti et al. 1990; O’Sullivan et al. 1996), and therefore photoabsorption both below and above the K-shell threshold could be investigated. However, only preliminary identifications of the 1\textit{s}→2\textit{p} resonances were possible due to the poor resolution of those experiments. Furthermore, their interpretation can be extremely complicated since (1) the ions are distributed over various charge states in both the ground and metastable states, (2) the presence of a plasma affects the energy levels, and (3) post-collision interactions can occur.

The most reliable data for the below-threshold 1\textit{s}→\textit{np} resonant absorption for carbon ions to date have been provided by third-generation synchrotron radiation experiments at the Advanced Light Source (ALS) on the positive-ion beamline (Schlachter et al. 2004; Scully et al. 2005; M"{u}ller et al. 2009). However, these measurements only investigated ionized carbon, not neutral C\textsubscript{i}. Furthermore, these experiments were restricted in photon energy range and did not span the entire photon energy range.

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region of the K edge but instead investigated only the 1s → 2p resonances in C II (Schlachter et al. 2004), the 1s → 2p and 1s → 3p resonances in C III (Scully et al. 2005), and the 1s → 2p and 1s → 3p resonances in C IV (Müller et al. 2009). The ion beams in those experiments (Schlachter et al. 2004; Scully et al. 2005) also contained an admixture of the metastable state in addition to the ground state. Although the experimental investigations were accompanied by a detailed R-matrix theoretical analysis (Schlachter et al. 2004; Scully et al. 2005; Müller et al. 2009), only cross section data for the 1s → 2p, 3p resonances were reported.

Thus, the only reliable photoabsorption data for carbon ions would appear to be the above-threshold IP cross sections (Reilman & Manson 1979) for the 1s → e p photoionization of C I–C IV and the below-threshold ALS experimental cross sections for the 1s → 2p, 3p photoexcitation of C III–C IV, along with the accompanying R-matrix results. In this paper, we present new R-matrix calculations for the photoabsorption of C I–C IV that cover the entire photon energy region of interest, namely, the below-threshold 1s → np photoexcitation of the entire Rydberg series (n → ∞) merging smoothly into the above-threshold 1s → e p photoionization, thereby treating the K-edge photoabsorption features correctly. The computed carbon and carbon-ion cross sections are then used to interpret the X-ray spectra from a high-quality Chandra observation of the blazar Mkn 421 and to determine relative carbon-ion abundances.

2. THEORETICAL METHODOLOGY

The specific processes of interest are the K-shell photoexcitation of the carbon-ion ground state,

\[ hν + 1s^22p^6 → 1s2lq^2np , \]

followed by two competing decay routes. First, there is participator Auger decay

\[ 1s2lq^2np → 1s2lq^2lq−1 + e− , \]

where the valence electron np takes part in the autoionization process; the decay width therefore scales as \( 1/n^2 \) and goes to zero near the K-shell threshold. There is also the more important spectator Auger decay

\[ 1s2lq^2np → 1s2lq^2lq−2np + e− , \]

where the valence electron np does not take part in the autoionization process, giving instead a decay width that is independent of \( n \). Spectator Auger decay is therefore the dominant decay route as \( n \to \infty \) and gives a smooth cross section as the K-shell threshold is approached; above each threshold, K-shell photoionization to the 1s2p\(^6\) states occurs instead. We note that for \( n = 2 \), there is no distinction between spectator and participator channels.

To account for photoionization to the participator channels, we use the standard R-matrix method (Burke & Berrington 1993; Berrington et al. 1995) and expand the total wave function in a basis consisting of free electron orbitals \( e^l \) coupled to each of the ground-state and singly excited 1s2lq\(^-1\) target wave functions, plus bound orbitals \( np \) coupled to the K-shell vacancy target wave functions 1s2p\(^6\). However, the infinite number of 1s2lq\(^-2\)np + e− spectator decay channels are impossible to include implicitly in such an R-matrix expansion; instead, they are accounted for via an optical potential approach (Gorczyca & Robicheaux 1999). The target energy for each closed channel 1s2lq\(^n\)p is modified within a multi-channel quantum defect theory approach as

\[ E_{1s2lq^2} → E_{1s2lq^2} + iΓ_{1s2lq^2}/2 . \]

where \( Γ_{1s2lq^2} \) is the 1s2lq\(^2\) → 1s2lq\(^2\) + e− Auger width. This enhanced R-matrix method was shown to be successful in describing experimental synchrotron measurements for Ar I (Gorczyca & Robicheaux 1999), O I (Gorczyca & McLaughlin 2000), and Ne I (Gorczyca 2000), and neon ions (Juett et al. 2006). We compute the 1s2lq\(^2\) Auger widths by applying the Smith time-delay method (Smith 1960) to the photoabsorption R-matrix calculation of the neighboring 1s2lq\(^-1\) carbon ion. Since 1s → 2p photoabsorption of the 1s2lq\(^-1\) ion gives an intermediate 1s2lq\(^2\) resonance, the subsequent Auger decay to the 1s2lq\(^2\) + e− channel can be analyzed to obtain the Auger width.

It is also important to obtain accurate target wave functions using a single orthogonal orbital basis, and this is problematic since orbital relaxation occurs when the 1s2lq\(^-1\) states are excited to the 1s2lq\(^2\) K-shell-vacancy states (the 2p electrons are now only screened by one, not two, 1s electron). We account for orbital relaxation by using additional pseudoorbitals as follows. A basis of physical 1s, 2s, and 2p orbitals is first constructed by performing Hartree–Fock calculations for the 1s2lq\(^-1\) ground states. Then, multiconfiguration Hartree–Fock (MCHF) calculations (Fischer et al. 1997) are performed for the 1s2lq\(^-1\) K-shell-excited states, including all configurations obtained from single and double promotions out of the 1s2lq\(^-1\) and 1s2lq\(^2\) states, using the six orbitals 1s, 2s, 2p, 3s, 3p, and 3d. Our computed R-matrix C I–C V target energies are shown in Tables 1–4, respectively, and compared to the currently recommended NIST values\(^4\) for the 1s2lq\(^-1\) singly excited states. To our knowledge, there are no experimental or theoretical values for the K-shell-excited 1s2lq\(^-1\) energies for comparison except for the 1s2s\(^\pm\) 2p\(^\pm\) (4P) state of C I. The energy of this state corresponds to the K-shell threshold in the photoabsorption of C I and was measured to be 296.07 ± 0.2 eV by Bruch et al. (1985), which is in good agreement with our predicted value of 296.096 eV.

We construct total wave functions by coupling an additional bound (np) or continuum (e p) electron orbital to the target wave functions. Standard R-matrix calculations were then performed including only the participator channels, and by investigating the behavior near the 1s2lq\(^-1\) resonances, the Auger widths of Equation (4) are determined. These R-matrix Auger widths are listed in Tables 5–7 and compared to multiconfiguration Breit–Pauli (MCBP) and multiconfiguration Dirac–Fock (MCFD) results. Given the Auger widths, the spectator Auger channels are also included in the optical potential R-matrix calculations for C I–C IV to yield cross sections with the correct resonance widths for \( n > 2 \).

We present R-matrix description can be summarized as follows for the photoabsorption of each ion 1s2lq\(^n\). A target-state expansion of the ground and singly excited states 1s2lq\(^n\)

\(^4\) http://www.nist.gov/physlab/data/asd.cfm
Note. The 1s2s2p(1P) energy of 20.9133 Ryd relative to the 1S 2s2p(1P) ground state of CNI corresponds to a K-shell threshold energy of 296.098 eV relative to the CNI ground state, which compares favorably to the experimental value of 296.07 ± 0.2 eV (Bruch et al. 1985).

Table 1
Energies (in Rydbergs) of the Cn Target States and the C1s Ground State

| State       | R-matrix | NIST |
|-------------|----------|------|
| 1s2s2p(1P)  | 0.0000   | 0.0000 |
| 1s2s2p(2P)  | 0.3814   | 0.3922 |
| 1s2s2p(2D)  | 0.7128   | 0.6828 |
| 1s2s2p(2S)  | 0.9950   | 0.8793 |
| 1s2s2p(1P)  | 1.0450   | 1.0083 |
| 1s2s2p(2P)  | 1.3104   | 1.2942 |
| 1s2s2p(2D)  | 1.4311   | 1.3711 |
| 1s2s2p(2S)  | 1.6792   | 1.5377 |

Table 2
Energies (in Rydbergs) of the Cn Target States and the C1s Ground State

| State       | R-matrix | NIST |
|-------------|----------|------|
| 1s2s2p(1P)  | 20.9133  |      |
| 1s2s2p(2P)  | 21.1651  |      |
| 1s2s2p(2D)  | 21.1899  |      |
| 1s2s2p(2S)  | 21.3351  |      |
| 1s2s2p(1P)  | 21.4977  |      |
| 1s2s2p(2P)  | 21.6968  |      |
| 1s2s2p(2D)  | 21.8446  |      |
| 1s2s2p(2S)  | 22.0355  |      |
| 1s2s2p(1P)  | 22.1103  |      |
| 1s2s2p(2P)  | 22.2898  |      |
| 1s2s2p(2D)  | 22.3180  |      |
| 1s2s2p(2S)  | 22.4901  |      |
| 1s2s2p(1P)  | 22.6795  |      |
| 1s2s2p(2P)  | 22.7300  |      |
| 1s2s2p(2D)  | 23.0860  |      |

Table 3
Energies (in Rydbergs) of the Cr Target States and the C1s Ground State

| State       | R-matrix | NIST |
|-------------|----------|------|
| 1s2s2p(1S)  | 3.5264   | 3.5197 |
| 1s2s2p(2P)  | 0.5903   | 0.5883 |
| 1s2s2p(2D)  | 21.3887  |      |
| 1s2s2p(2S)  | 22.0009  |      |
| 1s2s2p(1P)  | 22.2508  |      |
| 1s2s2p(2P)  | 22.4955  |      |
| 1s2s2p(2D)  | 22.5767  |      |
| 1s2s2p(2S)  | 23.0266  |      |

Table 4
R-matrix Auger Widths (in eV) for the 17 Cn Target States

| State       | R-matrix | MBCP | MCDF |
|-------------|----------|------|------|
| 1s2s2p(1P)  | 6.45E-02 | 6.61E-02 | 6.08E-02 |
| 1s2s2p(2P)  | 9.14E-02 | 1.16E-01 | 8.62E-02 |
| 1s2s2p(2D)  | 4.93E-02 | 5.19E-02 | 4.75E-02 |
| 1s2s2p(2S)  | 8.65E-02 | 1.02E-01 | 1.49E-04 |
| 1s2s2p(1P)  | 1.55E-02 | 2.06E-02 | 5.86E-02 |
| 1s2s2p(2P)  | 4.60E-02 | 6.42E-02 | 4.77E-02 |
| 1s2s2p(2D)  | 3.56E-02 | 4.87E-02 | 3.73E-02 |
| 1s2s2p(2S)  | 7.21E-02 | 9.64E-02 | 9.08E-02 |
| 1s2s2p(1P)  | 6.42E-02 | 7.77E-02 | 8.01E-02 |
| 1s2s2p(2P)  | 4.57E-02 | 7.15E-02 | 2.49E-02 |
| 1s2s2p(2D)  | 7.78E-02 | 1.18E-01 | 8.23E-02 |
| 1s2s2p(2S)  | 1.49E-02 | 1.25E-02 | 8.89E-03 |
| 1s2s2p(1P)  | 6.56E-02 | 1.01E-01 | 7.13E-02 |
| 1s2s2p(2P)  | 3.89E-03 | 6.83E-02 | 5.18E-02 |
| 1s2s2p(2D)  | 7.24E-02 | 1.08E-01 | 8.16E-02 |
| 1s2s2p(2S)  | 4.60E-02 | 6.69E-02 | 5.03E-02 |
| 1s2s2p(1P)  | 4.90E-02 | 1.36E-01 | 5.56E-02 |

Note. Also shown are level-averaged MBCP (Hasoğlu et al. 2006) and level-averaged MCDF widths (Chen & Craseman 1988).

and the core-excited states 1s2p is made using the 1s, 2s, and 2p physical orbitals, where CI with additional configurations obtained by promotions to the 3s, 3p, and 3d pseudoorbitals is also included. These pseudoorbitals are optimized so that the additional CI compensates for the relaxation of the core-excited states relative to the ground state. It is important to treat this relaxation correctly since we wish to study the entire 1s2pnp photoabsorption series. The CI-enhanced physical 1s2pnp photoabsorption target states are then coupled to an additional bound or continuum electron, which is spanned by an internally generated, large basis of R-matrix orbitals, to produce the final wave function. In order to account for the 1s2pnp → 1s2pnp+e− spectator Auger decay, an additional imaginary term is added to the core-excited energies, resulting in a broadening of the core-excited resonances. This approach is to be contrasted with the earlier R-matrix work on carbon ions (Schlachter et al. 2004; Scully et al. 2005; Müller et al. 2009), which focused on the lowest resonances. Those calculations...
Also shown are level-averaged MBCP (Gorczyca et al. 2006) and level-averaged MCDF (Chen 1986).  

Note. Also shown are level-averaged MBCP widths (Gorczyca et al. 2003) and level-averaged MCDF widths (Chen 1985) widths.

| State  | R-matrix | MCBP | MCDF |
|--------|----------|------|------|
| $1s2s^22p^2(3P)$ | 7.18E − 02 | 7.93E − 02 | 6.72E − 02 |
| $1s2s^22p^2(3P)$ | 5.46E − 02 | 5.30E − 02 | 4.76E − 02 |
| $1s2s(3S)2p^2(3P)$ | 1.10E − 02 | 1.38E − 02 | 2.47E − 02 |
| $1s2s(3S)2p^2(3D)$ | 4.76E − 02 | 5.17E − 02 | 4.29E − 02 |
| $1s2s(3S)2p^2(3P)$ | 9.07E − 02 | 1.14E − 01 | 1.13E − 01 |
| $1s2s(3S)2p^2(3S)$ | 2.61E − 02 | 2.39E − 02 | 2.17E − 02 |
| $1s2s(3S)2p^2(3P)$ | 4.64E − 02 | 5.92E − 02 | 4.91E − 02 |
| $1s2s(3S)2p^2(3P)$ | 1.70E − 02 | 1.17E − 02 | 7.96E − 03 |
| $1s2s(3S)2p^2(3S)$ | 7.46E − 02 | 7.98E − 02 | 8.36E − 02 |
| $1s2p^3(3D)$ | 5.76E − 02 | 7.15E − 02 | 6.08E − 02 |
| $1s2p^3(3S)$ | ... | ... | 1.17E − 06 |
| $1s2p^3(3D)$ | 5.99E − 02 | 7.19E − 02 | 6.02E − 02 |
| $1s2p^3(3P)$ | 3.56E − 02 | 4.19E − 02 | 3.67E − 02 |
| $1s2p^3(3P)$ | 3.60E − 02 | 3.90E − 02 | 3.53E − 02 |

Note. Also shown are level-averaged MBCP widths (Gorczyca et al. 2006) and level-averaged MCDF widths (Chen 1986).

Included physical orbitals up through $n = 3$ and additional target pseudostates of the form $1s^22l^m2l^-n^mT^l$, but did not correct for spectator Auger broadening since only the lowest resonances were investigated. The number of pseudostates was necessarily finite and therefore spanned only a subset of the infinite number of spectator Auger channels. Such a target description is thus not appropriate for the present study since the $1s2l^mnp$ resonances require an accurate $1s2l^m$ relaxed-core description and the spectator decay of the entire Rydberg series $n \to \infty$ must be treated accurately. The target description used here necessarily differs from that of the earlier R-matrix studies (Sclachtter et al. 2004; Scully et al. 2005; Müller et al. 2009), and we therefore expect to find slight differences in the photoabsorption cross section obtained using either approximate wave function, giving an estimate of the theoretical uncertainty.

### 3. CROSS SECTION RESULTS

Our results for the C I photoabsorption cross section, using both length and velocity forms of the dipole operator, are shown in Figure 1. For exact wave functions, the two results will be identical, and the excellent agreement between our two cross sections is an indication that we have obtained fairly accurate R-matrix wave functions. We find similar excellent agreement between length and velocity results for C II-C IV photoabsorption and therefore only show length results in the remainder of the paper. IP results are also shown in Figure 1, which are seen to be in good agreement with our R-matrix cross section above the K-shell threshold.

Our computed $1s2s^22p^2(4P)$ K-shell threshold at 296.10 eV is in good agreement with the experimentally observed values of 296.2 ± 0.5 eV by Bsgaard et al. (1978) and 296.07 ± 0.2 eV by Bruch et al. (1985). The discontinuity around 291.6 eV in the R-matrix results is due to the turnover of Auger broadening below $n = 3$ to prevent double counting of the Auger width of the $n = 2$ resonance (the $1s2s^22p^2$ resonances only decay to participator channels). This discontinuity of $1.1 \times 10^2$ Mb is very small compared to the large resonance features of $10^3$--$10^5$ Mb.

The importance of including spectator Auger decay channels via the optical potential approach can be seen in Figure 2. Our results are shown with and without the spectator broadening effect. Whereas the spectator-broadened results show the physically correct constant Auger width near threshold, the un-broadened results have widths that approach zero near threshold and are therefore impossible to resolve using a finite set of energy mesh points. Results are not shown for the lowest $1s2s^22p^2$ resonances since these are not affected by spectator broadening.

The K-shell cross section for C II is shown in Figure 3 for the entire $1s \to np$ photoabsorption resonance region and for the above-threshold $1s \to \epsilon p$ photoionization region, where it is seen to be in fairly good agreement with the IP results of Reilman & Manson (1979). We note that the IP results are tabulated on a sparse grid, and for C I are provided at photon energies of 270 eV, 300 eV, and 330 eV, so that the results shown here are straight-line interpolations and do not exhibit

![Figure 1](image1.png)

**Figure 1.** C I photoabsorption cross sections: R-matrix length and velocity results compared to the independent-particle results of Reilman & Manson (1979).

(A color version of this figure is available in the online journal.)

![Figure 2](image2.png)

**Figure 2.** C I photoabsorption cross sections for $n \geq 3$ without (black) and with (red) spectator Auger broadening effects.

(A color version of this figure is available in the online journal.)
the unsmooth energy dependence found in our $R$-matrix cross sections.

For C\textsc{ii}, there also exist experimental and earlier $R$-matrix results for the $1s \rightarrow 2p$ resonances (Schlachter et al. 2004). In that experiment, in addition to the C\textsc{ii} $1s^22s^22p(^2P)$ ground state, there was a $\approx 20\%$ $1s^22s^22p(^4P)$ metastable-state fraction, giving additional resonances not included in our calculations for Figure 3. Thus, we performed an additional $R$-matrix photoabsorption calculation from the metastable state, including all quartet, rather than doublet, total symmetries, and then added the ground and metastable cross sections together with weightings of 80\% and 20\%, respectively. These results are shown in Figure 4 along with the earlier results. For the two strongest $^2P$ and $^2D$ resonances, where the experimental resolution was 65 meV, we find good agreement with the experimental resonance positions, but both present and earlier $R$-matrix resonance strengths are found to be significantly greater than the measured strengths. The second set of experimental results was taken at 120 meV for the weaker resonances, and here we find that our resonance positions are in error by as much as 0.5 eV and our strengths are again greater than experiment.

The differences seen in Figure 4 between the two theoretical results and the experimental measurements highlight the sensitivity of describing low resonances, in particular, to the atomic basis. Two independent $R$-matrix calculations are able to get a similar strength and position for one of the two prominent resonances (the $^2D$) but a larger difference in strength and position for the other (the $^2P$). Furthermore, both theoretical strengths for this latter resonance are significantly greater than the experimental value. As we will see similar differences for C\textsc{iii} and C\textsc{iv}, it is worth addressing these discrepancies at this point.

In our $R$-matrix basis, we have tried to give a reasonable description of the target states—the C\textsc{iii} states here—both for the ground and singly excited $1s^22s^2$, $1s^22s2p$, and $1s2p^n$ states, by using Hartree–Fock physical orbitals, and for the core-excited $1s2s^22p$, $1s2s2p^2$, and $1s2p^n$ states, by including additional pseudoorbitals. It is important to give a reasonably good description for the $1s2s^22p$ state, in particular, since this describes the core to which the strong $1s2s^22pnp$ photoabsorption resonances are attached. We thus expect the $1s2s^22pnp$ photoabsorption resonances to be described comparably well for higher $n$ since we have the case of a diffuse $np$ valence electron moving in the long-range field of the unperturbed target. However, for lower resonance states, especially the $1s2s^22p$ state ($n = 2$), this is no longer the case, and the “valence” $2p$ electron screens the $1s2s^22p$ “target” and leads to a secondary relaxation of all the $2p$ electrons. Ideally, we could introduce additional pseudoorbitals optimized on the relaxed $1s2s^22p^2$ resonance states, but then the calculations become increasingly complex. Furthermore, we find that such a procedure converges the C\textsc{ii} resonance state more than the C\textsc{iii} target state, giving a resonance energy position that is then lower than experiment.

And the difference between our present results and the earlier $R$-matrix results shows that different methods for describing the target states give somewhat different positions and strengths, so that we can conclude that the differences seen between the two theoretical results here and in later comparisons—up to about 20\% in resonance strength and as much as 0.5 eV in resonance position—can be considered our theoretical uncertainty for the lowest resonances. For higher resonances, of course, we expect a better description, although there are no experiment results available for benchmarking purposes and we must rely strictly on theoretical photoabsorption cross sections. Regarding the comparison between theoretical and experimental results, we note that, in addition to the relative experimental error bars shown in Figure 4 and in subsequent figures, there is also a systematic uncertainty in the normalization of the absolute cross section, which differs depending on the measurement of each resonance region separately, and this could help explain the differences seen.

We also note that, as indicated in Figure 4 as well as in Table 1, our energy ordering of the two lowest $1s2s2p^1$ quartet states—the $^4S$ state being lower in energy than the $^4D$ state—is in contrast to the ordering given earlier (Schlachter et al. 2004), as might be deduced using Hund’s Rule. However, there are in fact two such $1s2s2p(^4S)$ states as opposed to only one $1s2s2p(^4D)$ state. The reason one of the $^4S$ states should appear lower than the $^4D$ state is that the $2p^3(^4S)$ subshell has a lower energy than the $2p^3(^4D)$ subshell, and, when coupled with the strongly interacting $2s$ electron, the lowest-energy states are then $2s2p^2(^4S, ^4S)$ and $2s2p^2(^4D, ^4D)$. These shells then interact weakly with the $1s$ electron, and therefore the lower $^4S$ state has a $2s2p^3(^4S)$ $n = 2$ shell, which is lower in energy than the only $^4D$ state, which has a $2s2p^3(^4D)$ $n = 2$ shell. The energy
ordering as reported in an earlier study (Schlachter et al. 2004) is the reverse of the present energy ordering.

The C\textsc{ii} photoabsorption cross section for the entire K-edge region is shown in Figure 5 and compared to the IP results above threshold, where good agreement is again obtained. Here, only the ground-state photoabsorption cross section is shown, and we find that the lowest resonances are the 1s2s2p\(^2\)P resonance at 294 eV, the weaker 1s2s2p3s\(^1\)P resonance at 315 eV, and the 1s2s2p3p\(^1\)P resonance at 323 eV. By including contributions due to photoabsorption of the C\textsc{iii} 1s2s2p\(^3\)P metastable state, additional triplet resonances can be populated. Results for the lowest 1s → 2p, 3p resonances from the mixture of the ground and metastable states are shown in Figure 6 and compared to experimental results and earlier R-matrix results (Scully et al. 2005). Similar to C\textsc{ii}, we find significant differences between the three results. However, both R-matrix photoabsorption strengths for the dominant 1s2s2p\(^1\)P resonance are now less than the experimental value (Scully et al. 2005), in contrast to the dominant 1s2s2p\(^2\)P resonance in C\textsc{ii}, for which the two theoretical results were greater than experiment. Our present R-matrix energy position for this resonance is in somewhat better agreement with experiment than the earlier R-matrix result.

The two theoretical results give about the same strengths and widths for the 1s2s2p\(^3\)P resonance, and these strengths are within the error bars of the experiment (the relative uncertainty is greater for this weaker n = 3 resonance), but the positions are about 0.2 eV lower than experiment. For the resonances that are excited from the metastable state, there is good agreement between both theoretical results and the experimental data for the strength and position of the 1s2s2p\(^2\)P resonance and for the neighboring 1s2s2p\(^3\)D state, except that our position is about 0.1 eV higher than experiment for the \(^3\)D state. The most disturbing comparison is for the 1s2s2p\(^2\)S state, where we find a resonance position almost 0.45 eV too high compared to the other results. Apparently, this particular resonance is the most poorly described in our metastable calculation, and we can find no reasonable explanation for this anomaly; however, our primary focus is to obtain photoabsorption cross sections from the ground state for modeling purposes, and we do not pursue this resonance further.

The cross section for C\textsc{iv} is shown in Figure 7. Here, the resonances are given by \(\hbar\nu + 1s^22s \rightarrow 1s2snp\), and there are no spectator Auger decay channels. Therefore, in order to resolve the \(n \rightarrow \infty\) narrowing resonances as threshold is approached, we artificially broadened the entire series with a spectator width of \(\Gamma = 0.013\) eV. This is less than the resolution of the ALS experimental measurements, which was given for the C\textsc{iii} (Schlachter et al. 2004), C\textsc{iii} (Scully et al. 2005), and C\textsc{iv} (Müller et al. 2009) as \(\Delta E \geq 0.046\) eV, or the astrophysical measurement we describe, which is given as \(\Delta\lambda = 0.023\) Å, or \(\Delta E \approx 0.017\) eV for \(E \approx 300\) eV. Here, we see two prominent series of resonances—the lower 1s2s\(^3\)S\(np\) series terminating at 363.4 eV and the 1s2s\(^1\)S\(np\) series terminating at 368.8 eV—giving rise to two K edges. Above the K edge, our results again agree well with the IP results.
For the branching ratio for autoionization versus radiative decay, is equal to the photoabsorption cross section multiplied by $C_{iv}$ as we have noted, there is no spectator Auger decay for the Auger width is much larger than the radiative width. However, the experimental results for the photoionization continuum is non-negligible, as was found in the joint experimental and theoretical work on C iv (Müller et al. 2009). Thus, in order to compare to experiment (for the lowest three resonances), we do not use an artificial spectator Auger width and then compute both the total photoabsorption cross section and the radiation-damped photoionization cross section (Robicheaux et al. 1995). These cross sections are compared to the ALS experimental results and the earlier $R$-matrix results (Müller et al. 2009) in Figure 8. We see first that radiation damping effects cause a non-negligible reduction in the strength of the $1s2s2p[(3\, P)]$ and $1s2s3p[(3\, P)]$ resonances, but essentially no reduction in the $1s2s2p[(1\, P)]$ resonance strength.

The earlier $R$-matrix calculations were computed for the total photoabsorption cross section and were performed in both non-relativistic $LS$-coupling and semi-relativistic intermediate-coupling (IC) approximations; the main difference seen between the two sets of results is a slight shift in resonance positions. Our resonance positions differ from the experimental values by $\approx \pm 0.1$ eV for the two lowest $1s2s2p$ resonances and by $\approx -0.2$ eV for the next lowest $1s2s3p$ resonance. In every case, the earlier $R$-matrix results obtained positions in somewhat better agreement.

The theoretical resonance strengths for the two lowest resonances are both comparable to the experimental measurements. However, for the $1s2s3p[(1\, P)]$ resonance, the experimental strength is much weaker than our theoretical results even when radiation damping is included. We note that the experimental systematic uncertainty for the lower two resonances is 20\% whereas it is 40\% for the $1s2s3p[(1\, P)]$ resonance, and this may help explain the larger differences seen between theoretical and experimental results for this latter resonance.

### 4. The C K Edge in the X-Ray Spectrum of Mkn 421

We have also compared our $R$-matrix photoabsorption cross sections with the absorption features in the C K-edge structure present in a Chandra LETG+HRC-S spectrum of the blazar Mkn 421. While the LETG+HRC-S instrument has a strong C K-edge feature arising from a polyimide filter approximately 2750 Å thick, there should be additional absorption signatures present from the line-of-sight absorption toward Mkn 421.

Chandra has observed Mkn 421 on several different occasions, but one observation made by the LETG+HRC-S on 2003 July 1 and 2 (ObsID 4149) caught the object in a particularly bright state and is of much higher quality. The observation and data are described in detail by Nicastro et al. (2005).

We retrieved standard pipeline-processed products from the Chandra archive and constructed effective areas for the overlapping spectral orders 1–10 using standard CIAO tasks. Subsequent analysis was performed using the Interactive Data Language-based Package for Interactive Analysis of Line Emission (PINToFAL; Kashyap & Drake 2000). The adopted continuum model was optimized to the region around the C K edge, ignoring the absorption edge structure. A power-law continuum with photon index $\Gamma = 2$ and interstellar medium (ISM) absorption corresponding to a neutral hydrogen column density of $N_H = 1.5 \times 10^{20}$ cm$^{-2}$ computed using the cross sections of Balucinska-Church & McCammon (1992) were adopted. These values are close (but not identical) to the values found by Nicastro et al. (2005); small differences can be ascribed to our optimization to the C K-edge region and to revisions in the instrument calibration between their and our analyses.

While we could obtain a good match to the observations over the continuum regions around the C K edge, this model systematically underpredicted the data in the 42–44 Å range by about

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**Figure 8.** Present $R$-matrix cross section vs. experimental and earlier $R$-matrix results (Müller et al. 2009) for the $1s \rightarrow 2p$, $3p$ resonances of C iv. Green curve represents the experimental data. Black and blue curves show previous $R$-matrix results in $IC$- and $LS$-coupling schemes, respectively. Red and magenta curves show the present $R$-matrix photoabsorption and photoionization results, respectively. All theoretical cross sections are convoluted with an FWHM Gaussian given by the experimental resolution; the $1s2s2p[(3\, P)]^2 P$ and $1s2s3p[(3\, P)]^2 P$ resonances are measured with a spectral resolution of 46 meV whereas the $1s2s2p[(1\, P)]^2 P$ resonance is measured with a resolution of 121 meV. (A color version of this figure is available in the online journal.)
Based on the comparison of the calculations, the offset between the two is the C
However, we especially note two aspects of the results. First, some revision before quantitative measurements can be made.

There are no obvious signs of significant C absorption in the vicinity of 43 Å in the observed spectrum that is reasonably close to 42.15 Å in the observed spectrum. Second, there is a weak absorption feature near 43 Å which is notoriously difficult task for X-ray instruments in the vicinity of the C K edge. We applied a smooth broad Gaussian-like correction to the effective area in order to ameliorate this effect. The resulting model fit is illustrated in Figure 9. While the fit is generally very good, there is a clear discrepancy near 43 Å. The Balucinska-Church & McCammon (1992) cross section for carbon is essentially that from the synthesis of Henke et al. (1982, 1993) combined with the C abundance of Anders & Ebihara (1982), and amounts to a simple step function. We computed a new ISM absorption cross section replacing the neutral and ionized C cross sections with those from our R-Matrix computations. The division of carbon among different charge states was adjusted by eye to obtain a good match to the data. This was achieved with a mixture of 20% C, 60% C, and 20% C. The resulting model spectrum folded through the instrument response is also illustrated in Figure 9. There are no obvious signs of significant C IV absorption in the data.

We do not place great weight on the C ion ratios used for the fit: the instrument calibration would appear to require some revision before quantitative measurements can be made. However, we especially note two aspects of the results. First, the C II resonance structure now provides a good match to the observations in the vicinity of 43 Å and we consider this a reliable detection of this species. To our knowledge, this represents the first X-ray identification of C II absorption in interstellar gas. Second, there is a weak absorption feature near 42.15 Å in the observed spectrum that is reasonably close to the C III 1s2s2p2(\ell P) resonance predicted by our R-Matrix calculations. The offset between the two is -0.05 Å or 0.35 eV. Based on the comparison of the R-Matrix resonance energy and synchrotron observations illustrated in Figure 9, an offset of 0.35 eV is much too large to be associated with uncertainties in the predicted resonance position. Instead, it is possible that HRC-S imaging nonlinearities could give rise to such a discrepancy. Line positions are generally expected to be better than 0.01–0.02 Å, but can occasionally be as far as 0.05 Å out of place. We stop short of identifying this absorption feature but draw attention to its possible interest for future study.

5%–15%. We ascribe this to uncertainty in the calibration—a notoriously difficult task for X-ray instruments in the vicinity of the C K edge. We applied a smooth broad Gaussian-like correction to the effective area in order to ameliorate this effect. The resulting model fit is illustrated in Figure 9. While the fit is generally very good, there is a clear discrepancy near 43 Å. The Balucinska-Church & McCammon (1992) cross section for carbon is essentially that from the synthesis of Henke et al. (1982, 1993) combined with the C abundance of Anders & Ebihara (1982), and amounts to a simple step function. We computed a new ISM absorption cross section replacing the neutral and ionized C cross sections with those from our R-Matrix computations. The division of carbon among different charge states was adjusted by eye to obtain a good match to the data. This was achieved with a mixture of 20% C, 60% C, and 20% C. The resulting model spectrum folded through the instrument response is also illustrated in Figure 9. There are no obvious signs of significant C IV absorption in the data.

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5. SUMMARY AND CONCLUSION

In order to study X-ray absorption features near the carbon K edge, we have computed photoabsorption cross sections for C–C IV. We use an R-matrix method with the inclusion of spectator Auger decay and treat both the 1s → np resonance absorption for all n → ∞ and the above-threshold 1s → ϵp. We find excellent agreement with IP results for the above-threshold cross section.

Below threshold, the only other existing cross sections available for comparison purposes are the experimental and earlier R-matrix results for the 1s → 2p, 3p photoionization of C–C IV (Schlachter et al. 2004; Scully et al. 2005; Müller et al. 2009). We find that our present theoretical results are in generally good agreement with the earlier R-matrix results for the resonance strengths and positions, differing in energy position by roughly 0.1 eV and in strength by at least 20%, even though a somewhat different atomic structure was used in each calculation. However, the experimental resonance strengths differ from our theoretical results by as much as ≈ 40%, which could be explained by considering the experimental uncertainty in the absolute cross section normalization.

Most importantly, we have provided a comprehensive set of carbon photoabsorption data for the entire photon energy region including all 1s → np resonances that are broadened due to spectator Auger decay and merge smoothly onto the 1s → ϵp above-threshold continuum, thus modeling the K-edge photoabsorption features correctly.

These computed data are of particular importance for absorption studies of cosmic gas. In turn, a more accurate description of the interstellar absorption near the C K edge in cosmic sources used as in-flight calibration standards should lead to refinements in the calibration of spectrometers such as the Chandra LETGS. Analysis of the LETGS spectrum of Mkn 421 has allowed us to identify interstellar absorption due to C II and estimate ion fractions of C I and C II for the first time using X-rays.

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REFERENCES

Anders, E., & Ebihara, M. 1982, Geochim. Cosmochim. Acta, 46, 2363
Balucinska-Church, M., & McCammon, D. 1992, ApJ, 400, 699
Berrington, K. A., Eissner, W. B., & Norrington, P. H. 1995, Comput. Phys. Commun., 92, 290
Bisgaard, P., Bruch, Dahl, P., Fastrup, B., & Rodbro, M. 1978, Phys. Scr., 17, 49
Bruch, R., Luken, W. L., Culberson, J. C., & Chung, K. T. 1985, Phys. Rev. A, 31, 503
Burke, P. G., & Bruch, K. A. 1993, Atomic and Molecular Processes : An R-matrix Approach (Bristol: Institute of Physics Publishing)

5 For example, Chandra Proposer’s Observatory Guide: http://cxc.harvard.edu/proposer/POG

Figure 9. Carbon K-edge region of the X-ray spectrum of the bright blazar Mkn 421 observed by the Chandra LETGS/HRC-S. The edge absorption is predominantly due to the polyimide UV-optical/ion blocking filter on the HRC-S instrument, although ISM absorption contributions are also present. Two fits to a power-law continuum model with photon index Γ = 2.0, absorbed by an intervening ISM corresponding to a neutral H column density of 1.5 × 1020 cm⁻², are shown. These differ significantly only in the carbon cross sections employed: the neutral C I cross section of Balucinska-Church & McCammon (1992); and C I, C II, and C III cross sections reported here. In the latter case, the C I ion fractions were 20% C I, 60% C II, and 20% C III. The effect of the C II resonances is clearly visible in the vicinity of 43 Å. (A color version of this figure is available in the online journal.)
