ERRATUM: “HIGH PRECISION K-SHELL PHOTOABSORPTION CROSS SECTIONS FOR ATOMIC OXYGEN: EXPERIMENT AND THEORY” (2013, ApJL, 771, L8)

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There was an error in the description of the supplementary online material in this Letter. Instead of a supplemental data (FITS) file associated with Figure 1, each of Figures 1–4 should have had a link to a machine-readable table containing data used to create that figure. The figures are reproduced here with the correct explanatory text and the associated machine-readable tables are available in the online journal.

Online-only material: color figures, supplemental data

Figure 1. Photoionization cross sections of O+, O2+, and O3+ produced by the decay of a 1s hole in atomic oxygen. The resonance lines represent the transitions 1s2s2p5(1P), 1s2s2p6(4P)np, and 1s2s2p5(2P)np with n = 3–6. The current resolving power of the monochromator was 4250 ± 400 (≈124 ± 12 meV) at a photon energy of 526 eV.

(A color version of the figure and a machine-readable table containing the data used to create this figure are available in the online journal.)
Figure 2. Atomic oxygen photoabsorption cross sections taken at 124 meV FWHM compared with theoretical estimates. The R-matrix calculations shown are from the RMPS method (solid black line, present results) convoluted with a Gaussian profile of 124 meV FWHM. Table 1 designates the resonances and their properties. (A color version of the figure and a machine-readable table containing the data used to create this figure are available in the online journal.)

Figure 3. (a) R-matrix (RMPS) cross sections (convoluted at 124 meV) compared with central field approximation results (Yeh 1993), (b) Cross sections (un-convoluted) from the RMPS (solid black line) and Optical Potential R-matrix calculations (solid red line). (A color version of the figure and a machine-readable table containing the data used to create this figure are available in the online journal.)
Figure 4. ALS experimental quantum defects with those obtained from theory. The RMPS results are the filled triangles, and solid circles represent the optical potential approach (Gorczyca & McLaughlin 2000; García et al. 2005).

(A color version of the figure and a machine-readable table containing the data used to create this figure are available in the online journal.)

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HIGH PRECISION K-SHELL PHOTOABSORPTION CROSS SECTIONS FOR ATOMIC OXYGEN: EXPERIMENT AND THEORY

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ABSTRACT

Photoabsorption of atomic oxygen in the energy region below the 1s−1 threshold in X-ray spectroscopy from Chandra and XMM-Newton is observed in a variety of X-ray binary spectra. Photoabsorption cross sections determined from an R-matrix method with pseudo-states and new, high precision measurements from the Advanced Light Source (ALS) are presented. High-resolution spectroscopy with E/ΔE ≈ 4250 ± 400 was obtained for photon energies from 520 eV to 555 eV at an energy resolution of 124 ± 12 meV FWHM. K-shell photoabsorption cross section measurements were made with a re-analysis of previous experimental data on atomic oxygen at the ALS. Natural line widths Γ are extracted for the 1s−12s2p4(3P)np3P and 1s−12s2p4(3P)np3P Rydberg resonances series and compared with theoretical predictions. Accurate cross sections and line widths are obtained for applications in X-ray astronomy. Excellent agreement between theory and the ALS measurements is shown which will have profound implications for the modeling of X-ray spectra and spectral diagnostics.

Key words: atomic data – atomic processes – ISM: abundances – photon-dominated region (PDR) – stars: Wolf–Rayet – Sun: X-rays, gamma rays

Online-only material: color figures, Supplemental data (FITS) file (tar.gz)

1. INTRODUCTION

The photoionization process is one of the important radiative feedback processes in astrophysics (Miyake et al. 2010; Stancil et al. 2010). The increase in pressure caused by photoionization can trigger strong dynamic effects, such as photoionization hydrodynamics. The challenge in combining hydrodynamics with photoionization lies in the difference in time scales between the two processes. Photoionization and photoabsorption processes play important roles in many physical systems, including a broad range of astrophysical objects as diverse as quasi-stellar objects, the atmosphere of hot stars, protoplanetary nebula, H II regions, novae, and supernovae. The Chandra and XMM-Newton satellites currently provide an abundance of X-ray spectra from astronomical objects; high-quality atomic data is needed to interpret such spectra (McLaughlin 2001; Müller et al. 2010; Sant’Anna et al. 2011; Foster et al. 2010; Gharaiabe et al. 2010; McLaughlin & Ballance 2013). Theoretical studies, recently made on atomic carbon and it ions, indicated that high quality atomic data are necessary to accurately model Chandra observations in the X-ray spectrum of the blazar Mkn 421 (Hasoglu et al. 2010; Gharaiabe et al. 2011).

In the soft X-ray region (5–45 Å), spectroscopy, including K-shell transitions for atomic elements such as, C, N, O, Ne, S, and Si, in neutral or low stages of ionization and L-shell transitions of Fe and Ni, are a valuable tool for probing the extreme environments in active galactic nuclei, X-ray binary systems, cataclysmic variable stars and Wolf–Rayet stars (McLaughlin 2001; García et al. 2009; Foster et al. 2010; Skinner et al. 2010; Müller et al. 2010; Gharaiabe et al. 2011; Sant’Anna et al. 2011), and the interstellar medium (ISM; García et al. 2011; Gharaiabe et al. 2011). Interstellar oxygen is found in both the gas and dust phases, although the exact molecular form of the dust remains unknown. Therefore an accurate understanding of the gas phase constituents is necessary in order to measure the residual molecular and solid-phase components (Costantini et al. 2012).

In the X-ray community, electron beam ion trap (EBIT) measurements (used for calibrating resonance energies), have been carried out for the inner-shell 1s → 2ℓ transitions in He-like and Li-like nitrogen ions (Beiersdorfer et al. 1999), Li-like, Be-like, B-like, and C-like oxygen ions (Schmidt et al. 2004; Gu et al. 2005). In EBIT experiments, the spectrum is contaminated and blended with ions in multiple stages of ionization, making spectral interpretation fraught with difficulties. Cleaner, higher-resolution spectra are obtained at synchrotron radiation facilities; Advanced Light Source (ALS), BESSY II, SOLEIL, ASTRID II, and Petra III. EBIT experiments have the advantage of the production of pure ground state populations of atoms or ions, extremely difficult to make with merged beams methods, routinely used at synchrotron radiation facilities.

Photoionization and photoabsorption cross sections used for the modeling of astrophysical phenomena has traditionally been provided by theory, as limited experimental data is available across a wide range of wavelengths. Until recently, the bulk of theoretical work has not been tested thoroughly by experiment (McLaughlin 2001; Müller et al. 2010; Foster et al. 2010; Gharaiabe et al. 2011; Sant’Anna et al. 2011). For atomic oxygen the availability of X-ray data on this system provided the motivation to perform theoretical K-shell photoionization investigations.

Inner-shell excitation processes occurring with the interaction of a photon on the 1s22s22p4 3P ground-state of atomic oxygen
produces strong resonances observed in the corresponding cross section (cf. Figure 2 and Table 1), through promotion of the 1s $\rightarrow$ np electron via the processes

$$hv + O(1s^22s^22p^3[3P^o]) \rightarrow O(1s^22s^22p^4[2,4]Pnp^3P^o)$$

giving competing decay routes namely,

$$O^+(1s^22s^22p^3[3S^o, 2D^o, 2P^o]) + e^-(k_f^2),$$

and

$$O^+(1s^22s^22p^4[3P, 1D, 1S]n\ell\ell' + e^-(k_f^2),$$

which the present theoretical approach attempts to simulate, where, $n = 2$–6 (observed in the experiment), and $k_f^2$ is the outgoing energy of the continuum electron with angular momentum $\ell$. K-shell photoionization contributes to the ionization balance in a more complicated way than outer shell photoionization. K-shell photoionization when followed by Auger decay couples three or more ionization stages instead of two in the usual equations of ionization equilibrium (Petruzzi & de Araújo 1994, 1997).

Early theoretical photoionization cross section calculations for K-shell processes on this complex performed by Reilman and Manson (Reilman & Manson 1979) used the Hartree–Slater wavefunctions of Herman and Skillman (Herman & Skillman 1963; Yeh 1993) and the Dirac–Slater wavefunctions (Verner

### Table 1

| Resonances (Symmetry) | Energy $(eV)$ | Energy $(eV)$ | $\mu$ | $\mu$ | $\Gamma$ $(meV)$ | $\Gamma$ $(meV)$ | Lifetime $\tau$ (fs) |
|-----------------------|--------------|--------------|-------|-------|-----------------|-----------------|---------------------|
| $(3P^o)$              | $(R$-matrix$^a)$ | Expt Theory Expt Theory Expt Theory Expt Expt Expt |
| 2$p^5$                | 526.83       | 526.79 ± 0.04 | 1.110 | 1.110 ± 0.003 | 150$^a$         | 148 ± 11$^b$      | 2.22 ± 0.17        |
| 3$p$                  | 541.23       | 541.19 ± 0.04 | 0.796 | 0.811 ± 0.023 | 143              | 167 ± 11         | 1.97 ± 0.13        |
| 4$p$                  | 542.70       | 542.68 ± 0.04 | 0.801 | 0.825 ± 0.063 | 97               | 125 ± 11         | 2.63 ± 0.23        |
| 5$p$                  | 543.23       | 543.23 ± 0.04 | 0.824 | (0.800 ± 0.29) | 70               | 119 ± 10         | 2.77 ± 0.23        |
| 6$p$                  | 543.52       | 543.51 ± 0.04 | 0.833 | (0.800 ± 0.29) | 80               | 196 ± 12         | 1.68 ± 0.10        |
| ...                   | ...          | ...           | ...   | ...           | ...              | ...              | ...                |
| 1$s^{-1}4P$           | 544.03       | 544.03 ± 0.04 | ...   | ...           | ...              | ...              | ...                |
| 3$s$                  | 545.97       | 545.83 ± 0.04 | 0.826 | 0.870 ± 0.015 | 187              | 196 ± 10         | 1.68 ± 0.10        |
| 4$s$                  | 547.48       | 547.45 ± 0.04 | 0.848 | 0.871 ± 0.045 | 127              | 128 ± 10         | 2.57 ± 0.20        |
| 5$s$                  | 548.04       | 548.04 ± 0.04 | 0.902 | (0.870 ± 0.105) | 102            | 156 ± 10         | 2.11 ± 0.14        |
| 6$s$                  | 548.55       | 548.33 ± 0.04 | 0.784 | (0.870 ± 0.201) | 110            | 157 ± 13         | 2.10 ± 0.17        |
| ...                   | ...          | ...           | ...   | ...           | ...              | ...              | ...                |
| 1$s^{-1}2P$           | 548.85       | 548.85 ± 0.04 | ...   | ...           | ...              | ...              | ...                |

**Notes.** Experimental and theoretical energies (eV), quantum defects $\mu$, and natural line widths $\Gamma$ (meV) for the two prominent Rydberg series are presented. Lifetimes, $\tau$ (fs), given for the resonance states were determined from the uncertainty principle. Bracketed values represent the ALS experimental energies (eV) and quantum defects obtained using an average value of $\mu$. The error in the calibrated photon energy is ±40 meV. Instrumental resolution of 3800 ± 150 (±135 ± 5 meV) was used for the Gaussian portion of the Voigt function when refitting the previous (Stolte et al. 1997) and 4250 ± 400 (±124 ± 12 meV) for the current ALS experimental data.

* R-matrix (RMPS), 1$s^{-1}2,4P$ series limit are the ALS measurements of Stolte and co-workers (Stolte et al. 1997).
* Experiment, resolution of 4250 ± 400 (±124 ± 12 meV), to fit the current ALS data.
* Multi-configuration-Hartree–Fock (MCHF), Saha (Saha 1994).
* Experiment, resolution of 3800 ± 150 (135 ± 5 meV), to refit the previous ALS data (Stolte et al. 1997).
* S-matrix method, Petrinic and de Araújo (Petrini & de Araújo 1994).
* Experiment, Wisconsin, Synchrotron Radiation Center (SRC), Krause and co-workers (Krause 1994; Menzel et al. 1996).
Figure 1. Photoionization cross sections of $O^+$, $O^{2+}$, and $O^{3+}$ produced by the decay of a $1s$ hole in atomic oxygen. The resonance lines represent the transitions $1s2s^22p^4(^1P\text{)}$, $1s2s^22p^6(^3P\text{)}$, and $1s2s^22p^6(^3P\text{)}$ with $n = 3$–6. The current resolving power of the monochromator was 4250 ± 400 (≈124 ± 12 meV) at a photon energy of 526 eV.

Photoionization cross sections of $O^+$, $O^{2+}$, and $O^{3+}$ produced by the decay of a $1s$ hole in atomic oxygen. The resonance lines represent the transitions $1s2s^22p^4(^1P\text{)}$, $1s2s^22p^6(^3P\text{)}$, and $1s2s^22p^6(^3P\text{)}$ with $n = 3$–6. The current resolving power of the monochromator was 4250 ± 400 (≈124 ± 12 meV) at a photon energy of 526 eV.

(A color version and FITS images of this figure are available in the online journal.)

et al. 1993). Photoionization cross sections determined from central field approximations, although excellent for high photon energies, yield unreliable results near thresholds (see Figure 3(a)), where resonance features dominate the cross sections (Yeh 1993; Gharaibeh et al. 2011).

State-of-the-art ab initio calculations for photoabsorption cross-sections and Auger inner-shell processes were first investigated on this system, using the standard R-matrix approach (McLaughlin & Kirby 1998) for modeling the resolved interstellar O K, Ne K, and Fe L-edge absorption spectra in the Chandra X-Ray Observatory Low-Energy Transmission Grating Spectrometer (LETGS) spectrum of the low-mass X-ray binary X0614+091 (Paerels et al. 2001). This work was extended using the optical potential technique (Gorczyca & McLaughlin 2000) to account for Auger broadening of resonances below the $1s^{-1}$ threshold and to analyze the high-resolution spectroscopy of the oxygen K-shell interstellar absorption edge in seven X-ray binaries (Juett et al. 2004). García and co-workers (García et al. 2005), using the optical potential method within the Breit–Pauli R-matrix formalism (Burke 2011), extended this work to the oxygen iso-nuclear sequence and to investigate the X-ray absorption structure of atomic oxygen in the ISM by analyzing XMM-Newton observations of the low-mass X-ray binary Sco X-1 (García et al. 2011).

2. EXPERIMENT

Cross sections for atomic oxygen K-shell photoionization were measured over the photon range 520 eV to 555 eV. Our new results were obtained on the undulator beamline 11.0.2 at the ALS, and previous measurements were performed on the bend-magnet beamline 6.3.2 (Stolte et al. 1997). The present experimental measurements have covered the complete K-shell region, in a single scan, rather than constructing the spectra piece-meal like as was done previously (Stolte et al. 1997). A resolution of 4250 ± 400 (≈124 ± 12 meV) at 526.8 eV, and a photon flux of over $10^{11}$ photons s$^{-1}$ was provided by BL 11.0.2 when using slit widths of 20 μm. The experimental apparatus has been discussed previously in detail (Angel & Samson 1980; Stolte et al. 1997, 2008).

Similar to our earlier results (Stolte et al. 1997), we used the Rydberg resonance features found in molecular oxygen near 541 eV to calibrate the photon energy scale, resulting in a maximum uncertainty of 40 meV. During double-bunch operations of the ALS, a Wiley–McLaren style time-of-flight mass spectrometer (Wiley & McLaren 1955), oriented with its axis parallel to the polarization vector of the incident synchrotron radiation, was used in conjunction with a microwave discharge system to determine the branching ratios for atomic oxygen at the $1s2s^22p^6(^3P\text{)}$ resonance.

Both the microwave on (O and O2 mixture) and off (O2) independent spectral scans were divided by the incident photon flux. The molecular contribution to the microwave on spectrum was removed by a scaled subtraction of a microwave off spectrum at the O2 : $1s \rightarrow 1\pi_g$ resonance (530.5 eV). Several residual peaks are created due to the molecular resonances being a few meV wider for the microwave on spectra. We surmise that this difference is probably due to the larger thermal motion of the gas molecules with the microwave discharge on. The scans were finally corrected by removal of the background produced by direct photoionization of the atomic oxygen valence shell. This was only necessary for $O^+$ or $O^{2+}$, considering that $O^{3+}$ sat on a zero background. We performed two coarse photon energy scans, one for each ion, covering the range between 500 and 600 eV. The $O^+$ or $O^{2+}$ signal produced by K-shell photoionization is superimposed on a nearly flat background caused by direct photoionization of the valence shell. This background contributed 35% and 8% to the total $O^+$ and $O^{2+}$ signals, respectively, just above the $1s^{-1}2p$ series limit. The independent ion specific photon energy scans could then be placed onto a relative scale (Masuoka & Samson 1980) by using the branching ratios ($O^+/TIY = 80.07\%$, $O^{2+}/TIY = 17.32\%$, and $O^{3+}/TIY = 0.026\%$, with TIY = total ion yield) measured with the time-of-flight mass analyzer on top of the $1s2s^22p^5(^3P)$ resonance.

Finally, the scans were placed onto an absolute scale (see Figure 1) by summing their values above the $1s^{-1}2p$ series limit and normalizing this sum to the difference of the cross sections above and below the oxygen K-edge (Stolte et al. 1997, 1998, 2008).

3. THEORY

The R-matrix with pseudo-states (RMPS) method (Burke 2011; Berrington et al. 1995; Robicheaux et al. 1995; Ballance & Griffin 2006) was used to determine our theoretical results. Cross section calculations were performed in LS-coupling retaining 910 levels (valence and hole-states) of the residual $O^+$ ion in the close-coupling expansion. Hartree–Fock 1s, 2s, and 2p (Clementi & Roetti 1974) and $n = 3$ pseudo-orbitals of the $O^+$ residual ion (included for core relaxation and correlations effects) were used, obtained by optimizing on the energy of the hole state; $3\delta$, $5\delta$, and $3\delta$ on $1s2s^22p^4$ including the important configuration $1s^22s^22p^33\delta^2P$ with
the multi-configuration-Hartree–Fock (MCHF) atomic structure code (Fischer 1991).

For the O(1s^2 2s^2 2p^4 3 P) bound state we obtained 14.0344 eV for the ionization potential using a triple electron promotion model, the NIST experimental value is 13.61806 eV, a discrepancy of ~3% or 416 meV. A double electron promotion model gave 13.82184 eV, a discrepancy of ~1.5%, or 204 meV, yielding closer agreement with the NIST tabulated value as the RMPS approach provides more highly correlated wave functions. In previous work, Gorczyca & McLaughlin (2000) obtained an underestimate of the ionization potential ~2.5%, or 338 meV compared to experiment, due to limited correlation included.

In the collision calculations for atomic oxygen, 20 continuum functions and a boundary radius of 7.27 Bohr radii was used. Two- and three-electron promotion scattering models were investigated giving similar results. The collision problem was solved using an energy grid of 2 x 10^{-7} Ryd (≈2.72 μeV) allowing detailed resolution of resonance features in the cross sections.

The peaks found in the photoabsorption cross section spectrum were fitted to Fano profiles (Fano & Cooper 1968) instead of the energy derivative of the eigenphase sum technique (Quigley et al. 1998; Ballance et al. 1999). Theoretical values for the natural line widths Γ (meV) are presented in Table 1 and compared with current and previous ALS measurements (Stolte et al. 1997) and with prior investigations.

4. RESULTS AND DISCUSSION

In the photon energy range (520–555 eV) explored, an intense structure is observed in the cross section between 520 eV and 550 eV, from the strong 1s → 2p transition in the atomic oxygen spectrum. Figure 2 shows our present experimental and theoretical results for the photon energy range of 520–555 eV illustrating all the additional 1s → np transitions (n ≥ 3) in the spectrum. Previous experimental measurements (Stolte et al. 1997) were actually measured at a photon energy resolution of 135 meV and not 182 meV, and current ALS measurements are at 124 meV FWHM. Convolution of the RMPS theoretical results with a Gaussian function of 124 meV FWHM was used to compare directly with the ALS measurements. Resonances observed in the experimental measurements were fitted with Voigt profiles to determine the natural line widths using a Gaussian function of 124 meV FWHM for each peak. The photon energy was calibrated to an energy uncertainty of approximately ±40 meV.

Previous measurements of Stolte and co-workers (Stolte et al. 1997) were re-analyzed with the present results. The measured spectra for O^+, O^{2+}, and O^{3+} production were fitted with the program WinXAS© of Thorsten Ressler, Hamburg, Germany (Ressler 1983) and its near edge X-ray absorption fitting routines. Due to an incomplete data set, previous measurements for O^{3+} (Stolte et al. 1997) were not fitted. In previous measurements (Stolte et al. 1997), a width of 231 meV was cited with a resolution of 182 meV. On refitting the previous results (Stolte et al. 1997) it was discovered that it was not possible to arrive at a proper fit with a resolution of 3000. Current multi-function fits, using Voigt and arctan functions, determined the resolution to be 3800 ± 150 (≈135 ± 5 meV). The 1s2s^2 2p^4 (3 P^0) 6 p and 1s2s^2 2p^4 (3 P^1) 6 p states cannot be properly fitted, since they are completely hidden.

Rydberg’s formula was used to determine the resonance energies, given by,

$$\epsilon_n = \epsilon_{\infty} - \frac{Z^2}{\nu^2}.$$  \hspace{1cm} (1)

Where, $\epsilon_n$ is the resonance transition energy, in Rydbergs, $\epsilon_{\infty}$ the ionization potential and the resonance series limit. The principal quantum number $n$, the effective quantum number $\nu$ and the quantum defect $\mu$ are related by $\nu = n - \mu$ (Seaton 1983; Hinojosa et al. 2012). Converting all quantities to eV, members of the Rydberg series are represented by

$$E_n = E_{\infty} - \frac{Z^2 R}{(n-\mu)^2}.$$  \hspace{1cm} (2)

$E_n$ is the resonance energy position, $E_{\infty}$ the ionization limit, $Z$ is the charge of the core (in this case, $Z = 1$), and $R$ is 13.6057 eV (Seaton 1983; Hinojosa et al. 2012).

In Figure 2 we present the experimental cross section measurements from the ALS taken at $4250 \pm 400$ (≈124±12 meV) resolution compared to our theoretical work. In the non-resonant region, above the K edge, at 550 eV, theory gives a value of 0.560 Mb and the ALS experimental measured value is 0.559 Mb, a discrepancy of 0.03%. Figure 2 shows the excellent agreement between theory and experiment over the entire energy region and Figure 3(a) illustrates the RMPS results with the central field approximation (Yeh 1993) results. Strong resonance features near the K-edge present in the state-of-the-art RMPS cross sections are absent from the central field calculations. In Figure 3(b), un-convoluted, RMPS cross sections with the optical potential $R$-matrix results (Gorczyca & McLaughlin 2000) are presented. Note that the discontinuity (≈538 eV) in the optical potential $R$-matrix cross section results absent from the RMPS calculations. Finally, Figure 4 compares quantum defects $\mu$ obtained from the RMPS and the optical potential methods (Gorczyca & McLaughlin 2000; García et al. 2005) with experiment.

Table 1 presents our experimental and theoretical results, for resonance energies, resonance strengths $\sigma_{\infty}$ (Mb eV), quantum defects $\mu$ and natural line widths $\Gamma$ (meV) with previous theoretical and experimental work (Stolte et al. 1997; Petriini & de Araújo 1994; Menzel et al. 1996; Saha 1994; Krause 1994). Table 1 includes the experimental values for the lifetime $\tau$ expressed in femto-seconds (fs), determined via the uncertainty principle ($\Delta E \Delta t = \hbar/2$).
peaks observed in the cross sections over the entire energy range investigated allowed a direct comparison with state-of-the-art R-matrix calculations to be made. The only limitation of the present theoretical model is apparent from Table 1 concerning the resonance strengths which might be addressed in the future with an extended pseudo-states basis within a Breit–Pauli approximation. Finally, the data is suitable to be incorporated into the astrophysical modeling codes CLOUDY (Ferland 2003), XSTAR (Kallman & Bautista 2001), and AtomDB (Foster et al. 2012).

The energy resolution on present day satellites, Chandra and XMM-Newton, is ~0.6 eV, a factor of 10 lower than available at current ground-based synchrotron radiation facilities, such as the ALS, SOLEIL, ASTRID II, BESSY II, or PETRA III, providing higher resolution and precision than obtained via satellites. There are also issues concerning the calibration of spectra obtained from satellites as previously highlighted. The ALS measurements have been calibrated to the resonance transition in molecular oxygen, which is known very accurately.

In contrast, observed spectra using the LETG on Chandra are calibrated to either theoretical calculations or EBIT measurements (Schmidt et al. 2004; Gue et al. 2005) for the $1s \rightarrow 2p$ resonance line in H-like, He-like oxygen, Li-like, or B-like oxygens ions (with all the ensuing complications and difficulties of ion identification). Given the high precision of our experimental and theoretical data we recommend that observational data concerning K-shell photoabsorption of atomic oxygen be calibrated to the present work.

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5. CONCLUSIONS

K-shell photoabsorption of atomic oxygen was investigated using the RMPS method along with current and previous high resolution experimental measurements made at the ALS. Resonance features observed in the cross sections for photon energies in the range 520–555 eV, are identified as $1s \rightarrow np$ transitions that are analyzed, natural line widths $\Gamma$ (meV) extracted, and lifetimes determined via the uncertainty principle. Excellent agreement (see Table 1) of theoretical estimates for the resonance parameters (resonance energies, natural line widths, and quantum defects) compared to experimental measurements is obtained with calculations for the ionization potential accurate to within 1.5% of experiment. We have delineated all of the resonances properties and made a detailed comparison of experiment with current and previous theoretical investigations. Earlier theoretical work (Gorczyca & McLaughlin 2000; García et al. 2005) made a limited comparison with experiment for the quantum defects of the two resonance series with only the Auger width of $1s2s^22p^53P^o$ state determined. The present ALS high resolution (124 meV FWHM) of all the resonance

![Figure 3](image1.png) Figure 3. (a) R-matrix (RMPS) cross sections (convoluted at 124 meV) compared with central field approximation results (Yeh 1993), (b) Cross sections (un-convoluted) from the RMPS (solid black line) and Optical Potential approach (Gorczyca & McLaughlin 2000; García et al. 2005). The RMPS results are the filled triangles, and solid circles represent the optical potential results. (A color version of this figure is available in the online journal.)

![Figure 4](image2.png) Figure 4. ALS experimental quantum defects with those obtained from theory. The RMPS results are the filled triangles, and solid circles represent the optical potential approach (Gorczyca & McLaughlin 2000; García et al. 2005). (A color version of this figure is available in the online journal.)
