

X-RAY RESONANCE OPACITY OF OXYGEN AND IRON IN AGN MCG–6-30-15

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ABSTRACT

Theoretical differential oscillator strengths related to monochromatic opacity due to K- and L-shell absorption from oxygen and iron ions are directly compared with the *Chandra* and *XMM-Newton* spectra of Seyfert 1 galaxy MCG–6-30-15 . We compute the highly resolved continuum with resonances due to O I - VI and Fe XVI. It is found that the KLn ($n \rightarrow \infty$) resonance series limits in O VI, and the lowest LMM resonance in Fe XVI, lie at the prominent $\sim 17.5\text{\AA}$ break in the observed spectra. We also calculate and identify, for the first time, the observed gap in spectral flux at 22-23 \AA in the *Chandra* spectra due to K \rightarrow L resonant absorption features from *all* O-ions O I - VI, potentially leading to abundance determination of several or all ionization stages; similar signature gaps may be predicted due to other elements. The precise atomic parameters are computed in the relativistic close coupling approximation using the Breit-Pauli R-matrix method. The new X-ray opacities might possibly distinguish between models of a dusty warm absorber, and/or gravitational redshift and broadening due to a massive black hole in MCG–6-30-15 .

Subject headings: X-Rays : general — Ultraviolet : general — atomic processes — line: formation, identification — radiation mechanisms: thermal

1. INTRODUCTION

The Seyfert 1 galaxy MCG–6-30-15 has been under extensive study with new and continuing observations from *Chandra* and *XMM-Newton*. The soft X-ray region exhibits a predominantly non-thermal continuum with ‘breaks’ or ‘spectral turnovers’ with anomalous widths and depths larger than expected due to lines or photoabsorption ‘edges’ (Branduardi-Raymont *et al.* 2000, Lee *et al.* 2001, Sako *et al.* 2001). The primary interest in MCG–6-30-15 stems from earlier *ASCA* observations of the hard X-ray spectrum that show the prominent 6.4 keV iron K_{α} line with a large redward component, interpreted as gravitational broadening of emission from the inner region of the accretion disc around a massive black hole (Tanaka *et al.* 1995). Similarly, the positions and widths of the soft X-ray features were interpreted as gravitational broadening and redshift of recombination emission of H- and He-like Oxygen, and other elements, by Branduardi-Raymont *et al.* (2000) using the *XMM-Newton* data. However, Lee *et al.* (2001) obtained higher resolution *Chandra* data with the HETG and explained the spectrum in terms of a ‘dusty warm absorber’ model, with Rydberg series of lines from highly charged oxygen and iron ions, without requiring relativistic emission. The HETG observations of MCG–6-30-15 show a prominent break or spectral turnover at $\sim 17.5 \text{ \AA}$, at the edges corresponding to line opacity due to higher members of the Rydberg series $1s^2 \rightarrow 1snp$ of O VII, and the onset of the Fe-L edges. Their model also includes Fe XVII and Fe XVIII lines in the shorter wavelength region $\lambda < 17.5 \text{ \AA}$. At 22.05 \AA Lee *et al.* identify resonant photoabsorption by a KLL resonance in O VI predicted earlier (Pradhan 2000), and a tentative identification of the O I resonance at $\sim 23 \text{ \AA}$. These observations appeared to corroborate the Lee *et al.* warm absorber model. However, whereas the Lee *et al.* model includes line opacity from O and Fe ions, it does not consider resonance opacity (with the exceptions noted above).

Recently Sako *et al.* (2002) have reported additional *XMM-Newton* RGS observations

and analysis, reconfirming the conclusions of Branduardi-Raymont *et al.* (2000) as to gravitational broadening in MCG–6-30-15 . The *XMM-Newton* RGS data samples the longer wavelength region beyond that of the *Chandra* HETG, where Sako *et al.* find considerable differences between the observed flux and the dusty warm absorber model proposed by Lee *et al.* They also find O IV and O V features, in addition to the O VI feature found earlier. Although the Sako *et al.* model considers opacity sources from lines and resonances of the identified species (including iron oxides), they note in particular that there is insufficient opacity of O and Fe at the $\sim 17.5\text{\AA}$ break, and that the Lee *et al.* model overestimates the flux compared to observations. Hence they conclude that the shape and magnitude of the observed features are inconsistent with photoelectric absorption, and required Fe and O abundances, and reaffirm the model with relativistically broadened Ly α lines of ionized C,N, and O in irradiated accretion discs of MCG–6-30-15 , as well as another Seyfert 1 galaxy Mrk 766.

The two particular aims of this paper are: (i) to demonstrate resonance opacity from O and Fe ions as a significant contributor at $\sim 17.5\text{\AA}$ (in addition to line opacity), and (ii) to identify inner-shell resonant K_{α} absorption features from all O-ions, O I - O VI, that manifest themselves as the oxygen signature gap at 22-23 \AA in MCG–6-30-15 . The general aim is to illustrate the level of detail and precision required for astrophysical models in order to model *Chandra* and *XMM-Newton* sources. Atomic parameters for line, resonant, and continuum absorption are computed using ab initio methods with relativistic fine structure. The calculated oscillator strengths and photoionization cross sections are related directly to the monochromatic opacity spectrum which, in turn, determines the emitted flux and absorption features.

2. THEORY AND COMPUTATIONS

Resonance opacity complements line and continuum opacity. The monochromatic absorption coefficient may be defined in terms the quantity *differential oscillator strength* $\frac{df}{d\epsilon}$ (e.g. Pradhan 2000, Nahar *et al.* 2001) which subsumes these forms of atomic opacity, including autoionizing resonances. We express the line (bound-bound) and the resonant \oplus non-resonant (bound-free) absorption coefficient in terms of $\frac{df}{d\epsilon}$

$$a^{b-b}(\epsilon) = N_i f = N_i \left(\frac{\pi e^2}{mc} \right) \left(\frac{2z^2}{\nu^3} \right) \frac{df}{d\epsilon}; \quad a^{b-f}(\epsilon) = N_i \sigma_{PI}(\epsilon) = (4\pi^2 \alpha a_o^2) \frac{df}{d\epsilon}, \quad (1)$$

and where N_i is the ion density, z is the ion charge, and ν is the effective quantum number. The differential oscillator strength $\frac{df}{d\epsilon} = (\nu^3/2z^2) f_{line}$ for line opacity, and $\frac{df}{d\epsilon} = (1/4\pi^2 \alpha a_o^2) \sigma_{PI}$, where f_{line} is the oscillator strength, and σ_{PI} is the photoionization cross section. The $\frac{df}{d\epsilon}$ thus enables equal representation in magnitude of the b-b and b-f absorption coefficients, and is the basic atomic quantity that determines monochromatic opacity. We compute the $\frac{df}{d\epsilon}$ for all ions under consideration from the oscillator strengths and photoionization cross sections obtained from elaborate and extensive relativistic close coupling calculations using the Breit-Pauli R-matrix (BPRM) method (Scott and Taylor 1982, Hummer *et al.* 1993, Zhang *et al.* 1999).

All atomic calculations reported in this work are new, and have been carried out using configuration interaction eigenfunction expansions for the seven core O-ions, O II - O VIII, and for Fe-ions Fe XVI, XVII, and XVIII. In addition to the bound-free results reported herein, line f -values are also calculated for O VI and O VII, and Fe XVI and Fe XVII, including transitions up to $n = 10$ levels. While the voluminous atomic data calculations are still in progress, and will be reported separately, we present the results pertaining to resonances in the K_α complexes of O I - VI, and L-shell complex of Fe XVI.

3. RESULTS

In order to focus on the atomic physics of the opacity in the spectral region of the $\sim 17.5\text{\AA}$ turnover in the MCG–6-30-15 spectra, and the identification of resonant absorption from K_α complexes of O-ions and the LMM complex of Fe XVI, we consider the $\frac{df}{d\epsilon}$ for the relevant ions as obtained from ab initio calculations. In this report we eschew any modeling or fitting. While the relative magnitude of opacities depends on the densities, temperatures, ionization fractions, abundances etc. in a model, the actual spectral features — in energies and shapes — should be basically the same as the detailed structure in $\frac{df}{d\epsilon}$.

Fig. 1 shows the K_α resonant complexes of oxygen, with inner-shell excitation in all O-ions O I - OVI. Photoabsorption cross sections are from the ground level, and the dominant components and the peak positions of resonances in each ion are shown. In fact each complex has several components; their positions may or may not coincide depending on the exact energies of the contributing angular and spin symmetries. For example, O I and O II show one single peak because the contributing final $J\pi$ symmetries all lie at the same energy (π refers to the parity of the electronic state). On the other hand resonances begin to spread out with ion charge in O III and O IV, which also present more complicated resonance structures. The ground level of O III, $1s^22s^2p^2(^3P_0)$, photoionizes into the $J = (1)^o$ continuum of $1s2s^22p^3$ with the three components shown. O V has only one final $J\pi(^1P^o)$ since the initial level is $1s^22s^2(^1S_0)$. The KLL O VI is a twin component system discussed in detail in earlier works (Pradhan 2000, Nahar *et al.* 2001; the latter work includes Li-like C IV, O VI, and Fe XXIV). However, the O VI resonance at 21.87\AA is about an order of magnitude weaker than the stronger one at 22.05\AA ; the latter was identified in the MCG–6-30-15 spectrum by Lee *et al.* (2001; see Fig. 2 bottom panel). Most of these results for O-ions have been obtained for the first time (prior works on O I and O II resonances are discussed in Paerels *et al.* 2001, and below). The calculations also

include the K_α resonant oscillator strengths $\bar{f}_r = \int_{\Delta E_r} (df/d\epsilon)d\epsilon$ values for all O-ions (to be presented later), that might potentially determine column densities for all ionization stages of oxygen.

Fig. 2(a) presents the $\frac{df}{d\epsilon}$ for O and Fe ions. The O VI and the Fe XVI results are shown including the background, whereas the O I - O V resonances are shown only around the peak values that would be manifest in the observed MCG–6-30-15 spectra (bottom panel). The observed absorption spectrum corresponds to the inverse of the opacity. Therefore in Fig. 2(b) we plot $(\frac{df}{d\epsilon})^{-1}$, analogous to the $1/\kappa(h\nu)$ term in the integrand of the Rosseland harmonic mean for stellar opacities (e.g. Seaton *et al.* 1994), where κ_ν is the monochromatic opacity. The calculated opacity spectrum matches rather closely the observed spectra, and the large resonant opacity due to inner-shell excitation of six O-ions, O I - O VI, results in the gap or window in the 22-23 Å region clearly discernible in the *Chandra* MCG–6-30-15 spectrum by Lee *et al.* (2001). As observed, the O I resonance brackets this region on the longer wavelength side at 23.5 Å, and the stronger component of the O VI KLL at 22.05 Å on the shorter wavelength side.

The spectral turnover or break at $\sim 17.5\text{Å}$ in Fig. 2 has been discussed by Sako *et al.* (2002) with respect to both *Chandra* and *XMM-Newton* observations. Their warm absorber model flux is overpredicted compared to observations due to ‘lack of O VII and Fe L opacity’ (Sako *et al.*, Fig. 11). Here we find that the highest O VI KL*n* resonance series limit, as $n \rightarrow \infty$ lies at 17.42 Å. The resonances, towards the longer wavelength side $\sim 17.5 - 17.8\text{ Å}$, converge to several $n = 2$ thresholds $1s2s(^3S_1, ^1S_0)$ and $1s2p(^3P_{0,1,2}, ^1P_1^o)$. Resonances in O VI, up to $n = 50$, have been fully resolved at about 70,000 energies with an effective quantum number mesh that enables equal resolution for each n -complex. The downward jump in the theoretical absorpton spectrum in $(\frac{df}{d\epsilon})^{-1}$ at $\sim 17.5\text{Å}$ (Fig. 2b) corresponds directly to the similar jump in the observed flux.

There are actually two discrete jumps as seen in Fig. 3. The enhancement is mainly due to the considerable oscillator strengths in the $1s \rightarrow np$ inner-shell resonant transitions, and occurs largely at the lower $1s2s(^3S_1, ^1S_0)$ thresholds. The increase due to the higher $1s2pns$ series limits $1s2p(^3P_{0,1,2}^o, ^1P_1^o)$ is much smaller. The wavelengths corresponding to these threshold span the range 17.74 (2^3S_1) - 17.55 ($2^1S_0, 2^3P_{0,1,2}^o$) - 17.42 ($2^1P_1^o$) \AA . The O VI resonant absorption cross section, as $\lambda \rightarrow 17.42 \text{\AA}$, rises by a factor of 28 above the background continuum cross section, approaching the $n = 2$ excitation thresholds of O VII from below. Of course this is also the energy region corresponding to line opacity from the O VII $1s^2 \rightarrow 1snp$ transitions (Lee *et al.* include up to $n = 5$ in their model shown in the bottom panel of Fig. 2).

Also close to the $\sim 17.5\text{\AA}$ break are the lowest two resonances due to $2p^53s^2$ LMM complex of Fe XVI. The first (stronger) LMM resonance lies at 17.38\AA , but the Fe XVI bound-free continuum also has an appreciable value at the $\sim 17.5\text{\AA}$ (the second LMM resonance is at 17.10\AA). Moreover, the opacity from the next Rydberg complex in Fe XVI at $\sim 0.82 \text{ keV}$ corresponds to the strong absorption feature in the *Chandra* MCG–6–30–15 spectrum (even higher n -complexes become weaker roughly as n^{-3}).

4. DISCUSSION

A few salient points and implications of the present work are discussed.

K- and L-shell resonant absorption from O and Fe ions, respectively, should be a significant contributor to the missing or unidentified X-ray opacity in the warm absorber models of MCG–6–30–15 by Lee *et al.* (2001) and Sako *et al.* (2002). However the crucial question — whether the additional resonance opacity is sufficient, or whether relativistic emission still needs to be invoked — depends on the details of the model. In particular

the ionic column densities and O:Fe abundances need to explain, for example, the required optical depth of ~ 0.7 at $\sim 17.5\text{\AA}$. Nonetheless, it appears that most if not all atomic features in the observed spectrum may be theoretically modeled.

It appears likely that the K_α resonances of all ionization stages of oxygen are present in the *Chandra* MCG–6-30-15 spectrum. However, this presents rather a challenge to model, since the plasma source must necessarily imply a widely varying extended environment and/or intervening matter along the line of sight to the AGN. Whereas the O VI resonance opacity spectrum bears a striking resemblance to the observed spectra at the $\sim 17.5\text{\AA}$, complementing O VII line opacity (Fig. 2), the two ionization stages may differ by an order of magnitude in temperature, depending on the preponderance of photoionization or coronal equilibrium (or a hybrid) of the $(e + \text{O VII}) \rightleftharpoons \text{O VI}$ system. We therefore suggest an observational study of the O VI UV $\lambda\lambda$ 1031,1038 \AA doublet, cross-correlated with the O VI X-ray resonant absorption features described herein. The O VI KLL doublet *absorption* resonances at $\lambda\lambda$ 22.05 and 21.87 \AA (Pradhan 2000) lie between the well known forbidden (‘f’ or ‘z’), intercombination (‘i’ or ‘x,y’), and allowed (‘r’ or ‘w’) *emission* lines of O VII due to transitions $2(^3S_1, ^3P_{2,1}, ^1P_1^o) \rightarrow 1(^1S_0)$ at $\lambda\lambda$ 22.101, 21.804, and 21.602 \AA respectively. To augment theoretical studies, new self-consistent cross sections and rates O VI/O VII/O VIII have been computed (Nahar and Pradhan, in preparation) using the same eigenfunction expansion for both photoionization and recombination, and a unified (e + ion) recombination scheme including both radiative and dielectronic recombination, in an ab initio manner using the relativistic BPRM method (e.g. Nahar and Pradhan 1995, Zhang *et al.* 1999). The accurate new O VII total and level-specific recombination rates and A-values, up to $n = 10$ fine structure levels, should generally help the study of recombination lines, such as the O VII ‘He β , γ , δ , ϵ ’ identified by Sako *et al.* (2002) in the *XMM-Newton* spectrum, and for which the model absorption widths are ‘severely overpredicted’. Fine structure collisional cross sections and rates for O VII have also been

recently computed including up to $n = 4$ levels (Delahaye and Pradhan 2002).

The shape of the oxygen gap in the observed flux at ~ 0.55 keV ($22\text{-}23 \text{ \AA}$) is similar to the one in the ~ 0.94 keV region where Lee *et al.* (2001) have identified a line from He-like Ne IX ($1s^2 - 1s2p$). Based on the present study, inner-shell excitation from *all* Ne-ions should contribute to a ‘neon gap’ in this region. However, this gap would overlay the much stronger Fe L-shell opacity at all energies higher than the spectral break at $\sim 17.5 \text{ \AA}$. Nonetheless, in general we might predict similar gaps due to other elements, such as carbon at ~ 0.3 keV, nitrogen at ~ 0.4 keV, neon at ~ 0.9 keV, and from inner-shell K_α resonances in iron in the 6.4 - 6.7 keV range (the K_α complex in He-like iron at 6.7 keV, and Li-like dielectronic satellites at lower energies, are discussed by Oelgoetz and Pradhan 2001). These gaps or windows due to K_α resonant excitation in all ionization stages of an element would lie close together in the X-ray, and should be discernible (subject to the total opacity in that region). We note that the tentative identification by Lee *et al.* (2001) of the O I resonance in MCG-6-30-15 appears to be slightly higher in energy than the present value, and previous experimental and theoretical values at $\sim 23.5 \text{ \AA}$ discussed by Paerels *et al.* (2001), who used the non-relativistic theoretical cross sections for O I computed by McLaughlin and Kirby (1998) to analyse interstellar X-ray absorption (the theoretical model spectrum was shifted by 0.051 \AA to match the measured centroid wavelength of the O I resonance). Our O II K_α resonance is about 0.08 \AA lower than inferred from experimental data; however, new calculations are in progress.

Line and resonance complexes are sometimes referred to as ‘unresolved transition arrays’ (UTA’s, e.g. Sako *et al.* 2002). The present work demonstrates that it may be necessary to highly resolve the UTA’s, and precisely calculate the resonance profiles and energies, to analyze the high resolution data from *Chandra* and *XMM-Newton*. Owing to the convergence of resonance series limits from below threshold, the inner-shell ionization

‘edges’ are *always* diffuse and exhibit redward broadening. The total resonance averaged photoabsorption cross section is an analytic continuation of the cross section from just above threshold; continuum lowering effects at resonance series limits should also be manifest under appropriate plasma conditions.

In Fig. 1 we have presented only the K_α photoabsorption cross sections from the ground level of O-ions. Excited fine structure levels of the ground LS term may also be significantly populated; resonances in these excited level cross sections will also contribute to the absorption spectrum. As mentioned, we are computing comprehensive datasets for line f -values and photoionization cross sections of O-ions and Fe XVI, XVII, and XVIII, that should provide a more complete description of oxygen K-shell opacity for $\lambda > 17.5 \text{ \AA}$, and iron L-shell opacity for $\lambda < 17.5 \text{ \AA}$ in the region covered by both *Chandra* and *XMM-Newton*.

5. CONCLUSION

Comparison of ab initio theoretical atomic parameters that determine the X-ray opacity of O and Fe with the high-resolution *Chandra* and *XMM-Newton* observations reveal some spectral features heretofore unobserved in laboratory or astrophysical sources. We note the following main conclusions:

- Inner-shell K_α resonances from all O-ions O I - OVI are identified and associated with the window observed in the X-ray flux at $\sim 22\text{-}23 \text{ \AA}$ — spectral signature of oxygen absorption from an ‘all-component’ (mainly) optically thin plasma. Column densities of all ionization stages may be obtained using the calculated resonance oscillator strengths \bar{f}_r , and should provide stringent constraints on parameters such as temperatures and ionization fractions in photoionization models.

- Resonance series limits in O VI, and LMM resonances in Fe XVI, should contribute significantly to the opacity at the spectral $\sim 17.5\text{\AA}$ break in the 17.4 - 17.7 \AA range, possibly accounting for the missing O and Fe opacity to resolve the discrepancy between the the relativistic redshift and broadening model, and the dusty warm observer model.

- In general, high precision resolution of resonances is essential for theoretical X-ray models to match the high-resolution spectra of *Chandra* and *XMM-Newton* , as astrophysical laboratories of fundamental atomic and plasma physics.

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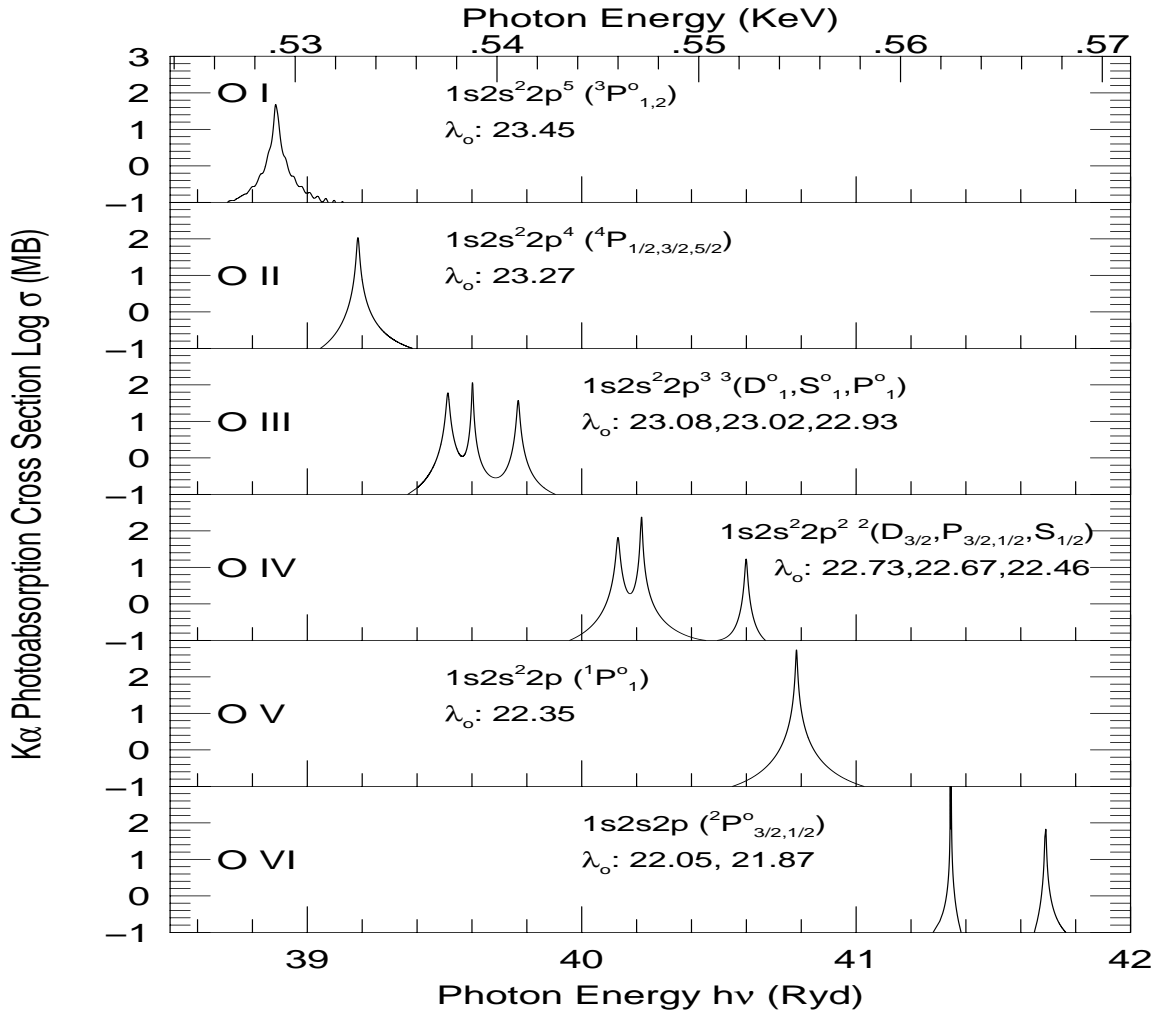


Fig. 1.— K_{α} photoabsorption cross sections of resonance complexes in Oxygen ions O I - O VI.

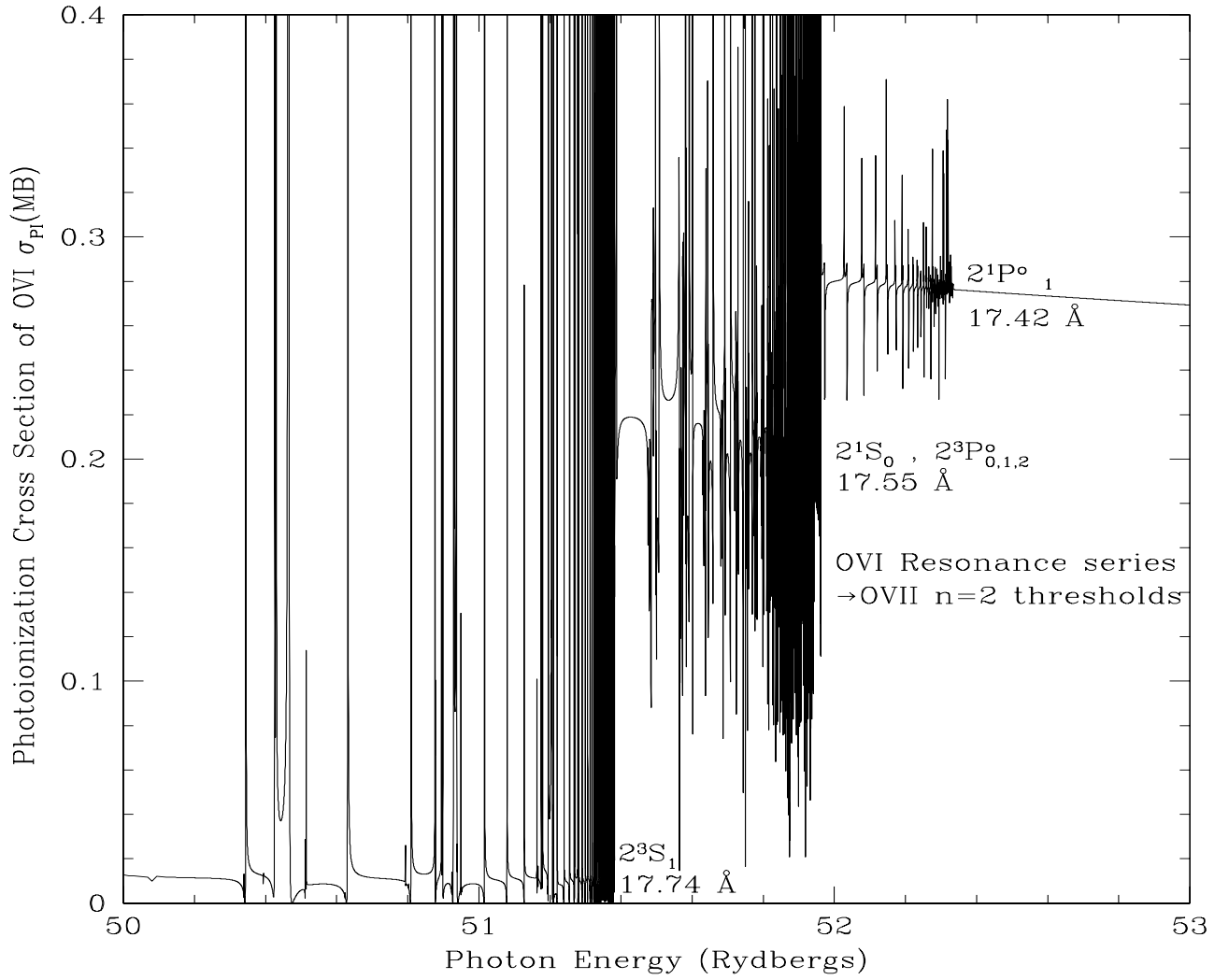


Fig. 3.— O VI resonances at the $n = 2$ O VII series limits: highly resolved photoionization cross sections in the ~ 0.7 keV region.