PHOTOIONIZATION MODELING OF OXYGEN K ABSORPTION IN THE INTERSTELLAR MEDIUM: THE CHANDRA GRATING SPECTRA OF XTE J1817-330

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ABSTRACT

We present detailed analyses of oxygen K absorption in the interstellar medium (ISM) using four high-resolution Chandra spectra toward the X-ray low-mass binary XTE J1817-330. The 11–25 Å broadband is described with a simple absorption model that takes into account the pile-up effect and results in an estimate of the hydrogen column density. The oxygen K-edge region (21–25 Å) is fitted with the physical warmabs model, which is based on a photoionization model grid generated with the xstar code with the most up-to-date atomic database. This approach allows a benchmark of the atomic data which involves wavelength shifts of both the K lines and photoionization cross sections in order to fit the observed spectra accurately. As a result we obtain a column density of $N_H = 1.38 \pm 0.01 \times 10^{21} \text{ cm}^{-2}$; an ionization parameter of $\log \xi = -2.70 \pm 0.023$; an oxygen abundance of $A_O = 0.689^{+0.015}_{-0.010}$; and ionization fractions of $O_1/O = 0.911$, $O_II/O = 0.077$, and $O_III/O = 0.012$ that are in good agreement with results from previous studies. Since the oxygen abundance in warmabs is given relative to the solar standard of Grevesse & Sauval, a rescaling with the revision by Asplund et al. yields $A_O = 0.952^{+0.020}_{-0.013}$, a value close to solar that reinforces the new standard. We identify several atomic absorption lines—Kα, Kβ, and Kγ in O I and O II and Kα in O III, O VI, and O VII—the last two probably residing in the neighborhood of the source rather than in the ISM. This is the first firm detection of oxygen K resonances with principal quantum numbers $n > 2$ associated with ISM cold absorption.

Key words: atomic data – atomic processes – ISM: general – stars: individual (XTE J1817-330) – X-rays: binaries – X-rays: general

Online-only material: color figures

1. INTRODUCTION

X-ray studies of interstellar absorption have the potential to provide information that is not accessible by other techniques. This includes the relative abundances of a wide range of ion stages of interstellar cosmic elements (e.g., oxygen) and the abundances relative to H and He of elements with atomic number $Z \geq 6$. X-ray absorption can also provide signatures of the binding of these elements in molecules or solids; the inner-shell electronic transitions are key diagnostics since the ionization state or chemical binding shifts the line energies by a predictable amount. The ongoing effort to explore and exploit this effect in interstellar studies involves accumulation of synthetic spectra for inner-shell absorption of ions and neutrals, based on both atomic calculation and laboratory experiment, in addition to testing them against available observed interstellar X-ray absorption spectra.

As part of the effort to accumulate the required atomic data, the atomic database of the xstar photoionization modeling code (Bautista & Kallman 2001) has been systematically improved in the past 10 years in order to study the K lines and edges in the high-quality X-ray astronomical spectra obtained from the Chandra and XMM-Newton satellite-born observatories. This database includes K-vacancy levels, wavelengths, $A$ values, radiative and Auger widths, and high-energy photoionization cross sections for complete isonuclear sequences with $Z \leq 30$ (see Palmeri et al. 2012 and references therein).

With this new database it has been possible, for instance, to estimate the model efficiency of iron K-line emission and absorption in terms of the ionization parameter and density (Kallman et al. 2004). It has been shown that the centroid of the Kα unresolved transition array, the Kβ energy, and the ratio of the Kα1 to Kα2 components are useful diagnostics of the ionization parameter. It was also found that the many strongly damped resonances below the K-ionization thresholds lead to edge smearing, which can certainly hamper the astrophysical interpretation of the absorption features. A synthetic spectrum has been modeled by Kallman et al. (2009) for the black hole X-ray transient GRO J1655-40 which constrains the odd Z element abundances ($11 \leq Z \leq 27$) and outflow parameters of the associated warm absorber. By analyzing the oxygen K-absorption structure in the interstellar medium (ISM) from the XMM-Newton spectrum of the low-mass X-ray binary Sco X-1, García et al. (2011) reproduced both the K edge and O I Kα absorption line, thus evaluating the impact of the atomic data on the interpretation of observations. In the present report we continue this work with a more stringent benchmark of the xstar atomic database, made possible by Chandra spectra of a low-mass binary displaying imprints of the ISM oxygen K absorption with higher resolution.
Juett et al. (2004) measured high-resolution spectra of the interstellar oxygen K shell absorption feature from seven X-ray binaries—Cygnus X-1, Cygnus X-2, 4U 1636-53, 4U 1735-44, GX 9+9, 4U 1543-624, and 4U 1820-30—using the Chandra High Energy Transmission Grating Spectrometer (HETGS). The oxygen column density $N_O$ was then calculated using the optical depth at 21.7 Å and the cross section at this wavelength assuming the oxygen abundance from Wilms et al. (2000). With this value, the hydrogen column density $N_H$ was then determined. The $1s$–$2p$ transitions of O ii and O iii were identified, finding ISM abundances for O ii and O iii relative to O i of $\approx 0.1$ and $\leq 0.1$, respectively. This became the first estimate of the O ii/O i and O iii/O i abundance ratios in the ISM.

By observing the oxygen K-shell edge toward galaxy clusters, Baumgartner & Mushotzky (2006) showed that the ISM hydrogen X-ray column density was in close agreement with the 21 cm radio value for columns less than approximately $0.5 \times 10^{21}$ cm$^{-2}$. For higher column densities, estimates by Baumgartner & Mushotzky were higher by as much as a factor of 2.5, indicating substantial absorption besides that due to neutral hydrogen (probably from clouds of molecular hydrogen). An average ISM oxygen abundance of 0.99 solar was found relative to the photospheric value ($^{8}\pm0.05$) by Asplund et al. (2004) which implied a high gas-to-dust ratio.

Pinto et al. (2010) reported a spectral model suggesting that, along the line of sight toward an X-ray source (GS 1826-2004) which implied a high gas-to-dust ratio. Oters, Baumgartner & Mushotzky (2006) showed that the ISM.

The oxygen column density $N_O$ of these three components span two orders of magnitude, where the cold gas contributed $90\%-95\%$, the warm gas $\sim 5\%-10\%$, and the hot gas $\sim 1\%$ to the total $N_H^{tot}$. Costantini et al. (2012) analyzed the ISM using the bright X-ray binary 4U 1820-30, concentrating on the mildly ionized cold gas where the model consisted of mildly ionized gas, dust, and mildly ionized outflowing gas. In the oxygen edge region, dust compounds were included which did not show features below 23.7 Å. Finally, oxygen was found to be overabundant by a factor of 1.23 solar.

In order to model the oxygen K-absorption features in the ISM with xstar, we need a Chandra spectrum with high counts. In the catalog of low-mass X-ray binaries by Liu et al. (2007), we found in XTE J1817-330 a suitable source with an average count number of $8 \times 10^6$ counts s$^{-1}$. Discovered by the Rossi X-Ray Timing Experiment (Remillard et al. 2006), XTE J1817-330 is a low-mass X-ray binary displaying a primary component which has an X-ray spectrum and variability behavior consistent with its identification as a black hole (Sala et al. 2007). Its location, $l = 359.81$ and $b = -7.99$ in Galactic coordinates, implies a line of sight in the Galactic center direction, a region that dominates the total mass of the Galaxy (Stasińska et al. 2012) providing a good opportunity to study the ISM absorption features. This source has been observed in different spectral ranges, namely the optical (Torres et al. 2006), near-infrared (D’Avanzo et al. 2006), radio (Rupen et al. 2006), and X-ray (Roy et al. 2011), Sala et al. (2007) fitted its X-ray spectrum finding an absorbing hydrogen column of $1.55 \times 10^{21}$ cm$^{-2}$ and identifying the following oxygen absorption lines: O i $\lambda$23.52 Å, O i $\lambda$23.55 Å, O iii $\lambda$23.13 Å, O i $\lambda$22.91 Å, and O vi $\lambda$21.60 Å. Gierliński et al. (2009) estimated a hydrogen column density of $N_H = 1.08 \pm 0.05 \times 10^{21}$ cm$^{-2}$, and Roy et al. (2011) investigated the timing characteristics in the spectra using a column of $N_H = 1.2 \times 10^{21}$ cm$^{-2}$.

The outline of the present paper is as follows. In Section 2, we describe the xstar xspec physical model which is used to obtain the final spectrum fits, in particular the details concerning its atomic database. The data reduction aspects of the observations, e.g., the pile-up effect, are reviewed in Section 3, while the results of the broadband fits and resolved absorption features are given in Sections 4 and 5. Section 6 is dedicated to comparisons of the hydrogen column density that allow an estimate of its reliability. Section 7 describes the oxygen column densities derived from our fits. Finally, the discussion and conclusions are presented in Section 8.

2. XSTAR/WARMABS

xstar is a code package designed to determine the physical conditions in partially ionized gases. It calculates the temperature, ionization, excitation, absorption, and emission due to neutral and all ionized species of elements with atomic number $Z \leq 30$. As many relevant physical processes as possible are taken into account, assuming a time stationary balance among them and a Maxwellian electron velocity distribution. Important processes for many problems relevant to X-ray astronomy include photoionization, electron impact collisional ionization and excitation, and radiative and dielectronic recombination. More complete descriptions of xstar and its atomic database are given by Kallman & Bautista (2001) and Bautista & Kallman (2001). In this work we employ the warmabs utility which allows for the calculation of xstar models within the widely used X-ray spectral fitting package xspec. It utilizes precalculated tabulations of the ion fractions and level populations in order to calculate synthetic emission and transmission spectra. It assumes that the gas responsible for emission or absorption has a uniform ionization and temperature throughout, although it is possible to superimpose two or more components and simulate a non-uniform situation.

2.1. Atomic Data

The K photoabsorption data sets for oxygen ions with electron numbers $2 \leq N \leq 8$ contained in the xstar atomic database were generated by García et al. (2005). Energies for both valence and K-vacancy fine-structure levels, transition wavelengths, $gf$ values, and radiative and Auger widths were computed with the atomic structure packages autostructure (Eissner et al. 1974; Badnell 1986, 1997) and hfr (Cowan 1981). Electron correlation effects were taken into account by means of configuration–interaction expansions within the $n \leq 3$ complexes, and relativistic corrections were included with a Breit–Pauli Hamiltonian. The accuracy of the theoretical level energies and wavelengths does not generally match that attained in experiments (see Table 1), and the scanty availability of measurements for the K shell of O ions with $N > 3$ limits the implementation of term-energy corrections and wavelength shifts that can be introduced in order to compensate for the theoretical shortcomings. Furthermore, as also shown in Table 1, experimental misassignments, such as that quoted by Gu et al. (2005) for O v i, are not uncommon. (The discrepancy in O iii is believed to be a typo.)

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8 http://heasarc.nasa.gov/lheasoft/xstar/xstar.html
9 http://heasarc.gsfc.nasa.gov/xanadu/xspec/
### Table 1
Comparison of EBIT and Theoretical Wavelengths (Å) for K Lines

<table>
<thead>
<tr>
<th>Ion</th>
<th>Lower Level (lJ)</th>
<th>Upper Level (lJ)</th>
<th>EBIT</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>O vi</td>
<td>1s²2s(1/2)</td>
<td>1s²2s²p(1/2, 3/2)</td>
<td>22.0194 ± 0.0016</td>
<td>22.00²</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>22.374 ± 0.008³</td>
<td>22.05⁴</td>
</tr>
<tr>
<td>O v</td>
<td>1s²2s²p(0)</td>
<td>1s²2s²p(1)</td>
<td>22.374 ± 0.003³</td>
<td>22.33³</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>22.370 ± 0.010⁵</td>
<td>22.35⁵</td>
</tr>
<tr>
<td>O iv</td>
<td>1s²2s²p²(1/2, 3/2)</td>
<td>1s²2s²p²(1/2, 3/2)</td>
<td>22.741 ± 0.005⁵</td>
<td>22.78⁸</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>22.73⁴</td>
<td>22.75⁵</td>
</tr>
<tr>
<td>O iii</td>
<td>1s²2s²p²(1, 2)</td>
<td>1s²2s²p²(1, 2)</td>
<td>22.071 ± 0.006⁶</td>
<td>23.08⁹</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>23.05⁴</td>
<td>23.07⁵</td>
</tr>
</tbody>
</table>

Notes.
* EBIT measurement (Schmidt et al. 2004).
* EBIT measurement (Gu et al. 2005).
* HULLAC calculation (Behar & Netzer 2002).
* R-matrix calculation (Pradhan et al. 2003).
* HFR calculation (García et al. 2005).

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High-energy photoionization cross sections in the K-edge region for oxygen ions were obtained by García et al. (2005) with HULLAC, the Breit–Pauli R-matrix suite of codes (Scott & Burke 1980; Scott & Taylor 1982; Berrington et al. 1987; Seaton 1987). A conspicuous effect in the resonance structure of these cross sections that must be treated in detail is Auger damping. It is the result of the dominant spectator KLL Auger decay channels of a photoexcited K-vacancy state, say,

\[
[1s]2p^{μ}np \rightarrow 2p^{μ−2}np + e^{-}
\]

\( (1) \)

\[
\rightarrow [2s]2p^{μ−1}np + e^{-}
\]

\( (2) \)

\[
\rightarrow [2s]2p^{μ}np + e^{-}
\]

\( (3) \)

over the participator Auger K\(L_{n}\) channels

\[
[1s]2p^{μ}np \rightarrow 2p^{μ−1} + e^{-}
\]

\( (4) \)

\[
\rightarrow [2s]2p^{μ} + e^{-}
\]

\( (5) \)

which leads to edge smearing by resonances with symmetric profiles of nearly constant width. They are handled within the R-matrix package by means of an optical potential (Gorczyca & Robicheaux 1999; Gorczyca & McLaughlin 2000). Again, the accuracy of the resonance energy positions is limited by the absence of measurements that would enable empirical adjustments of the many K-vacancy target thresholds (i.e., the series limits) in the close-coupling expansion.

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### Table 2
Chandra Observations Used in This Paper

<table>
<thead>
<tr>
<th>ObsID</th>
<th>Date</th>
<th>Exposure (ks)</th>
<th>Instrument</th>
<th>Grating</th>
<th>Label</th>
</tr>
</thead>
<tbody>
<tr>
<td>6615</td>
<td>2006 Feb 13</td>
<td>18</td>
<td>HETG-ACIS</td>
<td>MEG</td>
<td>Observation 1</td>
</tr>
<tr>
<td>6616</td>
<td>2006 Feb 24</td>
<td>29</td>
<td>HETG-ACIS</td>
<td>MEG</td>
<td>Observation 2</td>
</tr>
<tr>
<td>6617</td>
<td>2006 Mar 15</td>
<td>47</td>
<td>HETG-ACIS</td>
<td>MEG</td>
<td>Observation 3</td>
</tr>
<tr>
<td>6618</td>
<td>2006 May 22</td>
<td>51</td>
<td>HETG-ACIS</td>
<td>MEG</td>
<td>Observation 4</td>
</tr>
</tbody>
</table>

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3. OBSERVATIONS AND DATA REDUCTION

In Table 2 we list the specifications of the four observations of XTE J1817-330 obtained by Chandra using the HETGS in combination with the Advanced CCD Imaging Spectrometer (ACIS). The oxygen edge is accessible with the HETGS exclusively via the Medium Energy Gratings (MEG). Given the large flux of this source (\( F = 1350 \mu J \), integrated in the 2–10 keV energy range), these observations were taken in continuous clocking mode which significantly increases the temporal resolution in order to minimize the pile-up effect (Cackett et al. 2008). Pile-up is an inherent feature of CCD detectors, such as those of the ACIS instrument that occurs when two or more photons are detected as a single event possibly causing a deformation in the level and shape of the continuum (Miller et al. 2006b). It is stronger in the MEG than in the HEG due to the lower dispersion and higher effective area of the former.\(^{10}\) Although pile-up is usually not an issue near the oxygen edge, it may be for the continuum which is used to establish the hydrogen column density by fitting the 11–25 Å interval; hence, we consider the pile-up effect in this range by applying the correction model simple_agpile12_s1 (Hanke et al. 2009) before spectral fitting. Among the most popular computer packages for fitting X-ray data are xspec and isis, and we have used the latter (version 1.6.2\(^{11}\)) to include the pile-up model.

Even though the spatial resolution is reduced to one dimension when the continuous clocking mode is used, there is essentially no difference with the timed exposure mode in the background extraction or in the data reduction process. Hence, we have reduced the data sets using the standard CIAO threads.\(^{12}\) In some cases, the zero-order data were not telemetered; for these observations the zero-order position was then estimated by finding the intersection of the grating arms using the findzo algorithm.\(^{13}\)

Figure 1 shows the light curves of the four observations ObsID 6615, 6616, 6617, and 6618 in units of counts s\(^{-1}\).\(^{23}\)

\(^{10}\) http://cxc.harvard.edu/ciao/ahelp/acis_pileup.html

\(^{11}\) http://space.mit.edu/cxc/isis/

\(^{12}\) http://cxc.harvard.edu/ciao4.4/threads/gspec.html

\(^{13}\) http://space.mit.edu/cxc/analysis/findzo/
It can be seen that the average counts s\(^{-1}\) is approximately constant for all, and therefore we use the averaged spectra for this work. We have carried out the following spectral fitting procedure: first, each spectrum was rebinned with a 0.1 Å bin in order to fit the continuum in the 11–25 Å wavelength range so as to find the hydrogen column density using the TB\(_{\text{new}}\) model; then, the default spectral resolution was restored, and the oxygen edge region (21–24 Å) was analyzed with the warmabs model; then, the default spectral resolution was restored, and the model freezing the column density at the value obtained in the preceding step.

4. BROADBAND FIT

Following Yao & Wang (2006), we rebinned each spectrum with a 0.1 Å bin size throughout the spectral range to decrease the number of absorption lines and improve the broadband fit. We fitted the four observations simultaneously in the interval 11–25 Å using the simplegpile2(TB\(_{\text{new}}\)(powerlaw)) model, where simplegpile2 is a convolution model to account for pile-up effects and TB\(_{\text{new}}\) is an X-ray absorption model that includes abundances for elements from H to Ni (Wilms et al. 2000). Also we added Gaussians to fit the remaining absorption lines after rebinning. We used abundances specified in Wilms et al. (2000) and cross sections by Verner et al. (1996). The O, Ne, and Fe abundances were handled as free parameters, and for the analysis \(\chi^2\) statistics were employed. We fixed the absorption parameters in all the observations, and varied the power-law, pile-up, and Gaussian parameters for each case.

Figure 2 shows the fit in the interval 11–25 Å using the simplegpile2(TB\(_{\text{new}}\)(powerlaw)) model. Although the fit is carried out simultaneously for the four observations, they are plotted separately to improve clarity. Panels (a), (b), (c), and (d) correspond to observations ObsID 6615, 6616, 6617, and 6618, respectively (see Table 2). In each panel, black data points correspond to the observation, while the solid red lines represent the best-fit model for each case, and the base plots show the fit residuals in units of \(\chi^2\). Note the large residuals in the oxygen K-edge region, particularly in the neighborhood of the O i and O ii K\(_{\alpha}\) lines at \(\approx\)23.50 Å and \(\approx\)23.35 Å, respectively.

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

Figure 2. Chandra MEG spectra of the X-ray binary XTE J1817-330 simultaneously fitted in the 11–25 Å region using the TB\(_{\text{new}}\) model. (a) ObsID 6615. (b) ObsID 6616. (c) ObsID 6617. (d) ObsID 6618. See Table 2 for further details pertaining to these observations. In each panel, the black data points are the observations, while the solid red lines correspond to the best-fit models. Residuals are shown as histograms for each case in units of \(\chi^2\).
Table 3
Broadband Simultaneous Fit Parameters

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>TBNNew</td>
<td>$N_H$ ($10^{21}$ cm$^{-2}$)</td>
<td>1.66$^{+0.03}_{-0.04}$</td>
</tr>
<tr>
<td>TBNNew</td>
<td>Neon abundance ($A_{Ne}$)</td>
<td>2.258 ± 0.080</td>
</tr>
<tr>
<td>TBNNew</td>
<td>Iron abundance ($A_{Fe}$)</td>
<td>1.302 ± 0.050</td>
</tr>
<tr>
<td>TBNNew</td>
<td>Oxygen abundance ($A_O$)</td>
<td>1.178 ± 0.022</td>
</tr>
<tr>
<td>Power law</td>
<td>Normalization</td>
<td>9.416 ± 0.064$^a$</td>
</tr>
<tr>
<td></td>
<td>Photon index</td>
<td>1.545 ± 0.030$^a$</td>
</tr>
<tr>
<td>SimpleGpile2</td>
<td>$\beta$</td>
<td>0.050 ± 0.001$^a$</td>
</tr>
<tr>
<td></td>
<td>Rtot</td>
<td>21.286 ± 0.004</td>
</tr>
</tbody>
</table>

Notes. Abundances relative to the solar values of Wilms et al. (2000).

$^a$ ObsID 6615.
$^b$ ObsID 6616.
$^c$ ObsID 6617.
$^d$ ObsID 6618.

Fit results for the individual free abundances, column density, power law, and pile-up are presented in Table 3. The fit statistics give a reduced chi-square of $\chi^2 = 1.208$. Differences in the power-law parameters are due to the count numbers in each observation. We obtain abundances for O, Ne, and Fe higher than solar (Wilms et al. 2000), especially for Ne (a factor of two), and a column density of $N_H = 1.66_{-0.04}^{+0.03} \times 10^{21}$ cm$^{-2}$ which is somewhat larger than those estimated in other spectral fits and by measurements of the 21 cm line. This will be further discussed in Section 6.

The nonlinear pile-up convolution model simple_gpile2.s1 exponentially reduces the predicted count rate $R_l(\lambda)$ (in units of counts s$^{-1}$ Å$^{-1}$) according to

$$R(\lambda) = R(\lambda) \exp(-\beta R_{tot}(\lambda)),$$

where $R_{tot}(\lambda)$ is the total spectral count rate and $\beta$ is treated as a fit parameter. The model is only applicable to first-order grating spectra, although it employs information from the second- and third-order grating spectra. With this model we obtained an average $\beta = 0.050$ according to which the spectra have a pile-up degree greater than 25% for $14 \leq \lambda \leq 16$ Å with the highest value of $p = 42\%$ at $\approx 14.3$ Å for the observation with the largest number of counts (ObsID 6615). This value shows the need to include the pile-up effect in the 11–25 Å region to obtain a good fit. However, for all the observations, we have a pile-up degree lower than 5% in the 21–24 Å wavelength range which corresponds to the oxygen absorption region and, therefore, its effects were ignored.

5. ABSORPTION FEATURES

In order to identify all the absorption features present in the 21–25 Å wavelength region, we first applied a functional model consisting of a power law for the continuum and Gaussian profiles to describe the absorption lines. Figure 3 shows the spectral fit of the four Chandra MEG observations of XTE J1817-330 in the oxygen absorption region. Although shown in separate panels for clarity, the fit was performed simultaneously for the four observations. Nevertheless, the power-law parameters (photon index and normalization) are allowed to vary independently for each data set. Several absorption features are clearly observed, the most outstanding being the O i and O ii Kα lines. The base plot in each panel shows, in units of $\chi^2$, the fit residuals as a histogram. High residuals are found around 24.8 Å, and the model underestimates the number of photons around 23.2 Å.

Table 4 shows a list of the lines obtained with the functional fit including the centroid wavelengths derived from the Gaussian profile parameters. It also lists the wavelengths for the lines measured by Sala et al. (2007). Note that our wavelengths are within the error bars of the values reported by these authors, which are much larger given the lower spectral resolution of the XMM-Newton instruments. We obtain a reduced chi-square of $\chi^2 = 1.434$. The O i Kα is found at 23.502 ± 0.001 Å which has been previously declared to be of ISM origin (Sala et al. 2007). Furthermore, we have also detected four other O i absorption lines corresponding to resonances with higher principal quantum number $n$: two pairs of Kβ ($n = 3$) and Kγ ($n = 4$) resonances associated with the $^{14}$P and $^{14}$P K-hole core states. These are found at 22.884 ± 0.004 Å, 22.790 ± 0.001 Å, 22.686 ± 0.004 Å, and 22.609 ± 0.007 Å, respectively. In this set, only the first Kβ (belonging to the $^{14}$P core state) has been previously detected at 22.91 ± 0.03 Å in the XMM-Newton observation analyzed by Sala et al. (2007). This is the first firm detection of oxygen K resonances with $n > 2$ associated with ISM cold absorption.

The line at 23.358 ± 0.002 Å is also of ISM origin (Jeu et al. 2004) and corresponds to O ii Kα. As in the case of O i, resonances with $n > 2$ were also detected for O ii. These were found at 22.280 ± 0.003 Å and 22.101 ± 0.005 Å corresponding to Kβ and Kγ, respectively. Although the O iii Kσ resonance is a triplet, only two absorption features were detected at 23.104 ± 0.005 Å and 23.054 ± 0.001 Å while Sala et al. (2007) only found one line at 23.13 ± 0.09 Å identified as O iii Kσ. Finally, we have also located Kσ transitions for both O vi (22.022 ± 0.003 Å) and O vii (21.589 ± 0.003 Å), from which only the strongest of the two (O vii) was reported by Sala et al. (2007) at 21.609 ± 0.06 Å.
The functional fit described above illustrates the complexity of oxygen K absorption. There are (at least) two different regimes: a cold component of mostly neutral gas and a hot component with highly ionized gas. Previous studies have suggested a multiple-phase ISM; however, it is not clear if the two high-ionization lines from O\textsc{ii} and O\textsc{vii} are intrinsic to the source or if in fact arise in the ISM. Thus we direct our study to the cold phase. Furthermore, since cold absorption is not exclusively due to neutral oxygen, this means that a model such as TBnew will not completely represent the observed features. We have then simultaneously fitted the four exposures in the 21–25 Å wavelength range using the powerlaw*\textsc{warmabs} physical model. The advantage of using \textsc{warmabs} is that it contains the most recent atomic data for all the ions in the oxygen isonuclear sequence, thus enabling the fit of all the absorption features from O\textsc{i}, O\textsc{ii}, and O\textsc{iii}. While implementing this model, the column density is held fixed at the value obtained in the broadband simultaneous fit ($N_{\text{HI}} = 1.66 \times 10^{21}$ cm$^{-2}$). The ionization parameter and the oxygen abundance are treated as free parameters but the same for all observations, while the abundances of all the other chemical elements are held fixed at their solar values. The quantities describing the power law (photon index and normalization) are also taken as free parameters but independently for each observation.

Figure 3. Spectral fit of the Chandra MEG observations of XTE J1817–330 in the oxygen absorption region (21–25 Å) using a simple functional model (power law and several Gaussian profiles). (a) ObsID 6615. (b) ObsID 6616. (c) ObsID 6617. (d) ObsID 6618. The observed absorption features are interpreted as the neutral O K-edge ($\approx 23.1$ Å); the K$\alpha$, K$\beta$, and K$\gamma$ lines of O\textsc{i} ($\approx 23.50$ Å, $\approx 22.88$ Å, and $\approx 22.68$ Å, respectively); the K$\alpha$, K$\beta$, and K$\gamma$ lines of O\textsc{ii} ($\approx 23.35$ Å, $\approx 22.28$ Å, and $\approx 22.10$ Å, respectively); and the K$\alpha$ lines of O\textsc{iii}, O\textsc{vii}, and O\textsc{vii} ($\approx 23.10$ Å, $\approx 22.02$ Å, and $\approx 21.58$ Å, respectively). See Table 4 for more details.

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

Figure 4 shows the results of this fit. As before, we present for clarity the spectra with the best-fit model in separate panels, although the fit is performed simultaneously. Since most of the relevant absorption features in the spectra are due to neutral, singly, and doubly ionized O ions, the ionization parameter that describes the fit tends to be somewhat low: log $\xi = -2.729$. In this case, the \textsc{warmabs} model does not show any absorption due to O\textsc{vii}; therefore, this line is still represented with a Gaussian profile. We have found large residuals around most of the oxygen absorption features, the most prominent being around the O\textsc{i} and O\textsc{ii} K$\alpha$ lines. The fit statistics give a poor reduced chi-square of $\chi^2 = 1.769$ which forced us to revise the atomic database.

A close examination of the resonance positions from the photoabsorption cross sections used in \textsc{warmabs} in comparison with those obtained from the spectral fits with Gaussian profiles reveals the inaccuracies of the atomic data. Figure 5(a) shows with solid colored lines the atomic cross sections used in \textsc{warmabs} for O\textsc{i}, O\textsc{ii}, and O\textsc{iii} (García et al. 2005). Vertical dashed lines are placed at the positions of the absorption features found with the functional fit described above (see Table 4). A comparison shows that not only the positions of the O\textsc{i} and O\textsc{ii} K$\alpha$ resonances are displaced with respect to the observed data but also those with $n > 2$. The solid black line represents the experimental O\textsc{i} photoabsorption cross section measured.
Figure 4. Spectral fit of the Chandra MEG observations of XTE J1817-330 in the oxygen absorption region (21–25 Å) using a powerlaw*warmabs physical model. (a) ObsID 6615. (b) ObsID 6616. (c) ObsID 6617. (d) ObsID 6618. (A color version of this figure is available in the online journal.)

Figure 5. Comparison of the theoretical photoabsorption cross sections for O\textsc{i} (red), O\textsc{ii} (green), and O\textsc{iii} (blue) computed by García et al. (2005) that are implemented in the warmabs model. The black solid line is the laboratory measurement by Stolte et al. (1997) showing peaks of O\textsc{i} and O\textsc{ii}. The vertical dashed lines are placed at the wavelengths of the observed absorption lines (see Table 4). Panel (a) displays the original cross sections, while panel (b) shows the same curves after the wavelength shifts are applied to both O\textsc{i} and O\textsc{ii} (see the text for details). (A color version of this figure is available in the online journal.)

by Stolte et al. (1997; unfortunately, there are no laboratory measurements available for the other species) which displays a similar wavelength shift with respect to the observed resonance positions. This wavelength offset has been previously discussed by Juett et al. (2004) based on the Kα position observed in the Chandra spectra from several sources, all of which match the position we have found using Gaussian profiles. For O\textsc{i}, the comparison of the theoretical cross section with the laboratory measurement shows that, except for the Kα peak, all the other resonances agree very well. This implies that the relative position of the Kα with respect to the other resonances also needs to be adjusted. This is also the case for O\textsc{ii} since
the wavelength difference of the theoretical and observed Ka positions is not the same as those for the rest of the resonances of the same ion. Consequently, we have decided on the one hand to adjust the positions of the Ka resonances (which are treated as lines in warmabs), and on the other hand, to shift all the cross sections for both species so as to obtain the best possible agreement with the observed lines. The new positions for the O i and O ii Ka lines are 23.502 Å and 23.343 Å, while the cross sections were shifted toward shorter wavelengths by 0.033 Å and 0.079 Å, respectively. No correction was applied to the O iii curve since the observed lines are weaker, in addition to the fact that in this case the Kα resonance is a triplet. Figure 5(b) shows the atomic absorption cross sections after the wavelength corrections are applied. In other words, the Chandra observed line positions suggest not only that the theoretical resonance positions from García et al. (2005) must be adjusted, but also that the wavelength scale of the only available experiment for O i (Stolte et al. 1997) needs to be shifted by 33 mÅ.

Possible effects due to the instrument wavelength calibration, model uncertainties, and Doppler shifts due to motion of the gas in the ISM are important for accurate line identification. The instrumental resolution for the first-order spectra from MEG is $\Delta \lambda \sim 23$ mÅ, which is better than the largest shift required for our theoretical cross sections (33 mÅ). In fact, according to García et al. (2005), the uncertainties in the theoretical cross sections for O ions with electron occupancies $N \leq 4$ were estimated to be $\sim 50$ mÅ, comparable with the wavelength uncertainties in the laboratory measurements of Stolte et al. (1997). Assuming a velocity dispersion for the ISM of $\leq 200$ km s$^{-1}$ (Juet et al. 2004), the largest wavelength shift due to Doppler effects for the O i Kα is $\Delta \lambda = 14$ mÅ, which is smaller than the instrumental resolution. Hence, we can safely ignore the effects of ISM gas motion in the line of sight.

Figure 6 shows the fit results with warmabs after the theoretical line positions have been corrected, where the residuals are now significantly reduced and more evenly distributed. This is reflected in better fit statistics (reduced $\chi^2 = 1.245$) and a well-constrained ionization parameter (log $\xi = -2.699 \pm 0.023$) which is consistent with the low-ionization oxygen lines observed. As before, the O vii Kα resonance at 21.589 Å is not well represented with this model and must be fitted with a Gaussian profile. We have also noticed that the absorption feature at 22.022 Å is not entirely due to the O iii Kα resonance and is thus fitted with a Gaussian profile, confirming a blend of both O iii Kα and O vii Kα. In this final analysis, we also treated the column density value as a free parameter in order to increase the accuracy of the fit. We find a column density of $N_{\text{H}} = 1.38 \pm 0.1 \times 10^{21}$ cm$^{-2}$ that is lower than the value previously mentioned in connection with the broadband fit (see Section 4). The oxygen abundance obtained with the warmabs model is $A_O = 0.689^{+0.015}_{-0.010}$ relative to solar, also lower than the value for the best fit with TBnew ($A_O = 1.178 \pm 0.22$).

All the best-fit parameters of the warmabs are summarized in Table 5.
Table 5

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>warmabs</td>
<td>( N_H ) (10^{21} \text{ cm}^{-2})</td>
<td>1.38 ± 0.01</td>
</tr>
<tr>
<td>warmabs</td>
<td>Log ionization parameter (log ( \xi ))</td>
<td>-2.699 ± 0.023</td>
</tr>
<tr>
<td>warmabs</td>
<td>Oxygen abundance (( A_O ))</td>
<td>0.689^{+0.012}_{-0.010}</td>
</tr>
<tr>
<td>Power law</td>
<td>Normalization</td>
<td>2.384^a</td>
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<tr>
<td>Power law</td>
<td>Photon index</td>
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</tr>
<tr>
<td>Power law</td>
<td>Photon index</td>
<td>0.685^a</td>
</tr>
<tr>
<td>Power law</td>
<td>Photon index</td>
<td>2.479^b</td>
</tr>
<tr>
<td>Power law</td>
<td>Photon index</td>
<td>2.720^e</td>
</tr>
<tr>
<td>Power law</td>
<td>Photon index</td>
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<tr>
<td>Reduced chi-square</td>
<td>( \chi^2 )</td>
<td>1.245</td>
</tr>
</tbody>
</table>

**Notes.** Oxygen abundance relative to the solar value of Grevesse & Sauval (1998).

- ^a^ ObsID 6615.
- ^b^ ObsID 6616.
- ^c^ ObsID 8667.
- ^d^ ObsID 6618.

Table 6

<table>
<thead>
<tr>
<th>Method</th>
<th>( N_H ) (10^{21} \text{ cm}^{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>TBnew fit^a</td>
<td>1.66_{-0.04}^{+0.05}</td>
</tr>
<tr>
<td>warmabs fit^a</td>
<td>1.38 ± 0.1</td>
</tr>
<tr>
<td>21 cm survey ^b</td>
<td>1.58</td>
</tr>
<tr>
<td>21 cm survey ^c</td>
<td>1.39</td>
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<tr>
<td>Spectral model fit^d</td>
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<tr>
<td>Spectral model fit^e</td>
<td>1.2</td>
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<tr>
<td>Spectral model fit^f</td>
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<tr>
<td>Spectral model fit^g</td>
<td>1.0–3.0</td>
</tr>
<tr>
<td>Spectral model fit^h</td>
<td>1.08 ± 0.05</td>
</tr>
</tbody>
</table>

**Notes.**

- ^a^ Present work.
- ^c^ Kalberla et al. (2005).
- ^d^ Sala et al. (2007).
- ^e^ Rykoff et al. (2007), Gierliński et al. (2008), Roy et al. (2011).
- ^f^ Miller et al. (2006a).
- ^g^ Torres et al. (2006).
- ^h^ Gierliński et al. (2009).

6. HYDROGEN COLUMN DENSITY

Table 6 shows a comparison of the hydrogen column density obtained in this work with previous estimates including measurements using the 21 cm line. By means of the simultaneous broadband fit described in Section 4, we have obtained a column density of \( N_H = 1.66_{-0.04}^{+0.05} \times 10^{21} \text{ cm}^{-2} \) which is somewhat larger than those quoted in previous spectral fits. Miller et al. (2006a) reported a hydrogen column density of \( N_H = 8.8–9.7 \times 10^{20} \text{ cm}^{-2} \) using a 50 ks Chandra spectrum, a value smaller than those obtained from Galactic H\( i \) surveys, e.g., 1.58 \times 10^{21} \text{ cm}^{-2} (Dickey & Lockman 1990) and 1.39 \times 10^{21} \text{ cm}^{-2} (Kalberla et al. 2005). Using the equivalent widths (EWS) of several interstellar bands in the optical spectrum, Torres et al. (2006) found the column density to be in the range of \( N_H = 1–3 \times 10^{21} \text{ cm}^{-2} \). Moreover, both Rykoff et al. (2007) and Gierliński et al. (2008) gathered acceptable fits of several Swift X-Ray Telescope (XRT) spectra with a fixed Galactic column density of \( N_H = 1.2 \times 10^{21} \text{ cm}^{-2} \). Gierliński et al. (2009) used the same XRT spectra combined with data from UVOT (the Ultraviolet and Optical Telescope) to derive a column density of \( N_H = 1.08 \pm 0.05 \times 10^{21} \text{ cm}^{-2} \) from broadband spectral fits.

The agreement between TBnew and Sala et al. (2007) is around 7% despite the fact that their fits include data from XMM-Newton EPIC-Pn (0.6–10.0 keV), RGS1 (0.3–2.0 keV), and OM covering a much wider energy range; furthermore, they model the foreground absorption with warmabs, an older version of TBnew (Wilms et al. 2000). On the other hand, the present fits of the oxygen K region (21–25 Å) with the warmabs physical model yield a lower column density (\( N_H = 1.38 \pm 0.1 \times 10^{21} \text{ cm}^{-2} \)) than that derived from our broadband fit and TBnew. This discrepancy is expected due to the different atomic data sets involved, particularly since TBnew only includes the photoabsorption cross section for neutral oxygen. Taking into account the scatter of the previous column densities in the literature and the fact that we have adequately modeled the absorption features from O\( i \), O\( ii \), and O\( iii \), we would expect the value derived from warmabs to be more reliable than that from TBnew.

7. OXYGEN COLUMN DENSITY

In order to derive the O column density along the line of sight of XTE J1817-330, we have calculated the curve of growth for each of the oxygen K\( \alpha \) transitions using the atomic data from García et al. (2005), and EWs have been obtained using the functional fit described in Section 5. Table 7 shows a comparison between the present K\( \alpha \) EWs for O\( i \), O\( ii \), O\( iii \), O\( iv \), and O\( vii \) and those by Sala et al. (2007) for XTE J1817-330. EWs listed in Juett et al. (2004) for seven other sources are also included as well as those by Yao et al. (2009) for Cygnus X-2. For O\( i \) K\( \alpha \), our EW (51 \pm 5 mÅ) is around the lower limits in Sala et al. (2007) and Juett et al. (2004), and for O\( ii \) K\( \alpha \), the present value of 52 \pm 5 mÅ is within the range that Juett et al. (2004) associated with the ISM. However, we find the K\( \alpha \) lines in both O\( i \) and O\( ii \) to be saturated which could influence our derived EWs. Furthermore, the K\( \alpha \) EWs in O\( iii \), O\( iv \), and O\( vii \) are in good agreement with the values obtained by Juett et al. (2004), Sala et al. (2007), and Yao et al. (2009).

Table 8 shows a comparison of the oxygen column densities obtained from the EWs and the warmabs model fit. As previously mentioned in Section 5, for the ionization parameter found in our best warmabs fit, only O\( i \), O\( ii \), and O\( iii \) transitions are included.

Table 7

<table>
<thead>
<tr>
<th>Source</th>
<th>O( i ) K( \alpha ) (mÅ)</th>
<th>O( ii ) K( \alpha ) (mÅ)</th>
<th>O( iii ) K( \alpha ) (mÅ)</th>
<th>O( iv ) K( \alpha ) (mÅ)</th>
<th>O( vii ) K( \alpha ) (mÅ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>XTE J1817-330^a</td>
<td>51 ± 5</td>
<td>52 ± 5</td>
<td>16 ± 5</td>
<td>14 ± 5</td>
<td>54 ± 4</td>
</tr>
<tr>
<td>XTE J1817-330^b</td>
<td>70 ± 20</td>
<td>40 ± 20</td>
<td>30 ± 30</td>
<td>40 ± 30</td>
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<tr>
<td>Cyg X-2^c</td>
<td>67 ± 11</td>
<td>26 ± 17</td>
<td>9 ± 8</td>
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<td>Cyg X-2^d</td>
<td>50 ± 3</td>
<td>28 ± 6</td>
<td>11 ± 2</td>
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<tr>
<td>4U 1543-624^e</td>
<td>68 ± 11</td>
<td>41 ± 11</td>
<td>18 ± 5</td>
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<tr>
<td>4U 1820-30^f</td>
<td>70 ± 20</td>
<td>41 ± 17</td>
<td>20 ± 10</td>
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<tr>
<td>4U 1735-44^g</td>
<td>80 ± 30</td>
<td>40 ± 20</td>
<td>24 ± 10</td>
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<td></td>
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<tr>
<td>GX 9+9^h</td>
<td>80 ± 30</td>
<td>50 ± 19</td>
<td>27 ± 13</td>
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<tr>
<td>4U 1636-53^i</td>
<td>90 ± 30</td>
<td>60 ± 20</td>
<td>33 ± 13</td>
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<td>Cyg X-1 (ObsID 3407)</td>
<td>95 ± 17</td>
<td>20 ± 11</td>
<td>35 ± 15</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes.**

- ^a^ Present work.
- ^b^ Sala et al. (2007).
- ^c^ Juett et al. (2004).
- ^d^ Yao et al. (2009).
are taken into account in the model. As a reference, we have obtained improved statistics. However, it was realized that the pile-up effect must be taken into account in order to obtain reasonably reliable hydrogen column densities. This effect was treated adequately with the nonlinear pile-up convolution model simple_gpile2.sl, whereby the pile-up was estimated by fitting the continuum to be on average around 25%. The resulting hydrogen column density is $N_\text{H} = 1.66 \pm 0.03 \times 10^{21}$ cm$^{-2}$, which is somewhat ($< 7%$) higher than those from Kalberla et al. (2005) and Sala et al. (2007), the former obtained from 21 cm data.

The absorption features in the oxygen region (21–25 Å) were first picked up with a functional model (power law and Gaussian profiles) which yielded Kα lines of O i, O ii, O iii, and O vii previously observed by Sala et al. (2007), but for the first time, also K resonances of O i and O ii with principal quantum number $n > 2$. These line identifications at least confirm a two-phase plasma with both neutral (mostly) and highly ionized components. In the present work we have been mainly concerned with the former. In this respect, since neutral oxygen is not the sole charge state responsible for the cold oxygen absorption, the four exposures are then simultaneously fitted with a representative physical model referred to as warmabs, which contains the atomic data for the oxygen isonuclear sequence computed by García et al. (2005). In this step, the hydrogen column density is held fixed at the previously determined value of $N_\text{H} = 1.66 \times 10^{21}$ cm$^{-2}$, while the ionization parameters and oxygen abundance are treated as free parameters. A detailed comparison of this model with observations brings forth the inaccuracies of the atomic data, which led us to introduce wavelength shifts in both the Kα line positions and photoabsorption cross sections of O i and O ii.

The scope of this corrective procedure is severely limited by the general poor availability of laboratory data for the oxygen inner shell, but it certainly leads to improved fits and statistics, in particular, to a well-constrained ionization parameter of $\log \xi = -2.699 \pm 0.023$ consistent with the absorption lines observed. In order to further improve the fit, the column density is allowed to vary resulting in a more reliable value ($N_\text{H} = 1.38 \pm 0.1 \times 10^{21}$ cm$^{-2}$) which is within 13% of previous estimates (Kalberla et al. 2005; Sala et al. 2007). Furthermore, the fit yields an oxygen abundance of $A_\text{O} = 0.689_{-0.010}^{+0.015}$ and ionization fractions of $O_\text{i}/O = 0.911$, $O_\text{ii}/O = 0.077$, and $O_\text{iii}/O = 0.012$. Regarding the oxygen abundance, it may be clarified that the quoted value is given relative to the solar standard (8.83 ± 0.06) of Grevesse & Sauval (1998). If it is
rescaled to the recently revised standard by Asplund et al. (2009) of 8.69 ± 0.05, then an ISM abundance (A₀ = 0.952^{+0.020}_{-0.013}) close to solar is obtained which is in excellent accord with the averaged value by Baumgartner & Mushotzky (2006), and can be included as further support for the solar abundance revision. Moreover, our ionization fractions are in good agreement with those found by Juett et al. (2004) of O ii/O i ≈ 0.1 and O iii/O i < 0.1.

The functional fit allows us to derive oxygen column densities by means of a curve-of-growth method using the EWs for each of the observed Kα absorption lines, which can then be compared with the values obtained from the warmabs fit. Even though we find by both methods a relatively consistent total column density (5.71 \times 10^{17} \text{ cm}^{-2} in the curve of growth and N = 6.41 \times 10^{17} \text{ cm}^{-2} in the warmabs model fit), the O i/O ii ratio for the Kα lines is significantly lower (an order of magnitude) in the former. This is attributed to the high saturation magnitude) in the former. This is attributed to the high saturation

Evidence for this includes observed depletions of atomic oxygen or solids (dust). It is expected that these phases comprise a significant fraction of the total oxygen column in the ISM. The evidence for this includes observed depletions of atomic oxygen along many lines of sight relative to certain elements (Jenkins 2009; Yao et al. 2009; Whittet 2010), together with observations of molecular features in other wavelength bands. An example of a potentially detectable signature of such material is the K resonance of the CO molecule expected at a rest wavelength of 23.21 Å (Barrus et al. 1979). This line is separated from the nearest feature we clearly detect by approximately 100 mÅ, which can be compared with the magnitude of the wavelength shifts we adopt in order to get acceptable fits, the largest of which is 33 mÅ. Therefore, we conclude that the existing atomic absorption data are not sufficiently certain to mask the presence of this molecular signature. The search for molecular and solid features in X-ray spectra remains of great interest, both as tests of the atomic data and of models for the ISM.

We believe that the present benchmark has produced an improved version of the warmabs model that can now be used for a more extensive and reliable study of oxygen K photoabsorption toward other X-ray sources. This will be the next step of the current study where the oxygen abundance variations in the ISM are certainly of interest. In a similar fashion, we also intend to evaluate the Ne and Fe edge regions for ongoing physical model refinement.

Part of this work was carried out by Efraín Gatuzz during attendance of the Committee On Space Research (COSPAR) Capacity Building Workshop in San Juan, Argentina in 2011 July, and visits in 2011 August to the Laboratory of High Energy Astrophysics, NASA Goddard Space Flight Center, Greenbelt, Maryland, USA, and in 2012 February–March to the European Space Astronomy Centre (ESAC), Madrid, Spain, the latter funded by the COSPAR Fellowship Program. Warm hospitality and tutelage at these institutions are kindly acknowledged, in particular, from Andy Pollock and Carlos Gabriel at ESAC. We also thank Michael Nowak from MIT for useful discussions relating to the pile-up model and tss implementation.

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