THE KINEMATICS AND PHYSICAL CONDITIONS OF THE IONIZED GAS IN MARKARIAN 509. I.
CHANDRA HIGH ENERGY GRATING SPECTROSCOPY

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ABSTRACT

We observed the Seyfert 1 galaxy Mrk 509 for \( \sim 59 \) ks with the Chandra high-energy transmission gratings, simultaneously with \( HST/STIS \) and \( RXTE \). Here we present a detailed analysis of the soft X-ray spectrum observed with Chandra. We measure strong absorption lines from He-like Ne and Mg and from H-like N, O, and Ne. Weaker absorption lines may also be present. The lines are unresolved except for Ne x \( \lambda \) \( 12.134 \) and Ne \( \text{ix} \) \( 1s^2-1s2p \) \( \lambda 13.447 \), which appear to be marginally resolved. The profiles are blueshifted with respect to the systemic velocity of Mrk 509, indicating an outflow of \( \sim 200 \) km s\(^{-1}\). There is also a hint that the profiles may have a velocity component near systemic. The soft X-ray spectrum can be described in remarkable detail with a simple, single-zone photoionized absorber having an equivalent neutral hydrogen column density of \( 2.06 \pm 0.45 \times 10^{21} \) cm\(^{-2}\) and an ionization parameter of \( \log \xi = 1.76 \pm 0.13 \) (or \( \log U = 0.27 \)). Although the photoionized gas almost certainly is comprised of matter in more than one ionization state and may consist of several kinematic components, data with better spectral resolution and signal-to-noise ratio would be required to justify a more complex model. The UV data, on the other hand, have a velocity resolution of \( \sim 10 \) km s\(^{-1}\) and can easily detect eight kinematic components, covering roughly the same velocities as the X-ray absorption profiles. Even though the X-ray and UV absorbers share the same velocity space, the UV absorbers have a much smaller column density and ionization state. We show that models of the X-ray data do not predict significant UV absorption and are therefore consistent with the UV data. Finally, we do not detect any soft X-ray emission lines.

 Subject headings: galaxies: active — galaxies: individual (Markarian 509) — galaxies: Seyfert — techniques: spectroscopic — ultraviolet: galaxies — X-rays: galaxies

1. INTRODUCTION

X-ray and UV absorption and emission by photoionized circumnuclear gas in type 1 Seyfert galaxies is a key observational diagnostic. While it has been possible to study the UV absorption with a velocity resolution of \( \sim 10 \) km s\(^{-1}\), the kinematics of the X-ray absorber observed with CCDs (such as those aboard \( ASCA \)) could be studied only with a velocity resolution greater than \( 10,000 \) km s\(^{-1}\). Inadequate spectral resolution, combined with a lack of simultaneity between X-ray and UV observations, has resulted in major uncertainties in the dynamics, physical state, location, and geometry of the X-ray and UV absorbers, as well as the relation between the two. The launch of Chandra and \( XMM-Newton \) began a new era in the study of X-ray photoionized circumnuclear gas. The energy resolution of the Chandra transmission gratings is currently the best available in the 0.5–10 keV band and is as high as \( \sim 280 \) km s\(^{-1}\) at 0.5 keV. High-resolution X-ray spectroscopy with Chandra now allows the gas kinematics to be studied seriously for the first time, and the detection of individual absorption and emission lines can now place very strong constraints on the ionization structure of the gas.

The existence of warm, or partially ionized, X-ray-absorbing gas in type 1 active galactic nuclei (AGNs) was first suggested by \( Einstein \) observations of QSO MR 2251+178 (Halpern 1984). Subsequently, \( ROSAT \) and \( ASCA \) showed this to be a common phenomenon, present in roughly \( 50\%-60\% \) of type 1 AGNs, and studies focused on the measurements of the O \( \text{vi} \) and O \( \text{vii} \) absorption edges, which appeared to be the most prominent features in these low to moderate resolution spectra (Nandra & Pounds 1992; Fabian et al. 1994; Reynolds 1997; George et al. 1998). High resolution grating observations with Chandra have since been used to study the X-ray warm absorbers in several Seyfert 1 galaxies (Collinge et al. 2001; Lee et al. 2001; Sako et al. 2001a; Pounds et al. 2001; Kaastra et al. 2002; Kaspi et al. 2002; T. Yaqoob, B. McKernan, I. M. George, & T. J. Turner 2003, in preparation). Discrete, narrow absorption features (FWHM \( < 2000 \) km s\(^{-1}\)), often unresolved, are found to be typically blueshifted, with outflow velocities ranging from a couple hundred to a couple thousand kilometers per second relative to systemic. Moreover, in some cases multiple velocity components have been identified (Collinge et al. 2001; Kaspi et al. 2002; Kaastra et al. 2002). There are typically fewer features in emission than absorption (e.g., Kaastra et al. 2002; Kaspi et al. 2002). UV-absorbing gas in Seyfert 1 galaxies was first observed with \( IUE \) (Ulrich 1988). Multiple discrete kinematic components
to the UV absorbers have been observed, and it has been suggested that the X-ray absorber is associated with one or more, but not necessarily all, of the UV components (e.g., Mathur, Elvis, & Wilkes 1995, 1999). Observations with the improved sensitivity and resolution of HST/STIS and FUSE have since shown that ~60% of Seyfert 1 galaxies exhibit intrinsic UV absorption and that multiple kinematic components are common (Crenshaw et al. 1999).

At present, models of the X-ray absorbers span a wide range in distance from the central ionizing source, from winds originating at the accretion disk (Elvis 2001), out to the putative (parsec scale) molecular torus (e.g., the multimperature wind model of Krolik & Kriss 2001), and beyond, to the narrow-line region (e.g., Ogle et al. 2000). In addition, for two particular Seyfert 1 galaxies observed by XMM-Newton (MCG –6-30-15 and Mrk 766), it has been proposed that relativistically broadened soft X-ray lines from an accretion disk can account for some of the spectral features traditionally attributed to a warm absorber (Brandaudi-Raymont et al. 2001; Sako et al. 2001a). However, Lee et al. (2001) have argued that the Chandra grating data, for MCG –6-30-15 at least, can be modeled with a dusty warm absorber without the relativistic emission lines. One thing is clear, however: all of the models must stand up to the scrutiny of an increasingly large body of results as the results of new observational campaigns become available.

The purpose of the present paper is to present the results of such new campaign, namely, simultaneous Chandra HETGS, HST/STIS, and RXTE observations of the luminous $L_{2-10\text{keV}} \approx (1.3-2.6) \times 10^{44}$ ergs s$^{-1}$; Weaver, Gelbord, & Yaqoob 2001)7 Seyfert 1 galaxy Mrk 509 (z = 0.0344; Fisher et al. 1995). Mrk 509 has been studied extensively in the UV and by every major X-ray astronomy mission since HEAO-1 A-2. Being so bright and exhibiting interesting absorption structure in the UV (e.g., Kriss et al. 2000) and X-ray bands (e.g., Pounds et al. 1994, 2001; Reynolds 1997; George et al. 1998; Perola et al. 2000), Mrk 509 makes an excellent candidate for this kind of study. The driving principles behind our campaign were to measure, with the highest spectral resolution available, the X-ray and UV absorption features simultaneously in order to eliminate uncertainty due to variability and to measure the hard X-ray continuum simultaneously with the highest throughput available (i.e., with RXTE) in order to compensate for the poor efficiency of the Chandra gratings at energies above ~2 keV. In the present paper we focus on the soft X-ray spectroscopy results; detailed results from the UV data are presented in a companion paper (Kraemer et al. 2003, hereafter Paper II). Our campaign was also designed to measure the narrow and broad components of the Fe K line and associated Compton-reflection continuum, but these results are reported elsewhere (Yaqoob et al. 2002).

The paper is organized as follows. In § 2 we present the data and describe the analysis techniques. In § 3 we discuss gross features of the X-ray spectrum, including the intrinsic continuum form, and interpret the data in the context of historical, lower spectral resolution CCD data. In § 4 we qualitatively discuss the discrete X-ray spectral features before describing detailed spectral modeling. In § 5 we describe in detail the modeling of the X-ray spectrum using the photoionization code XSTAR. In § 6 we compare our results with those from a previous XMM-Newton grating observation by Pounds et al. (2001). In § 7 we discuss the relationship between the X-ray and UV absorbers. Finally, in § 8 we summarize our conclusions.

2. OBSERVATIONS AND DATA

We observed Mrk 509 with Chandra (simultaneously with HST/STIS and RXTE) on 2001 April 13–14 for a duration of ~59 ks, beginning at UT 08:01:31. The Chandra data were reprocessed using CIAO, version 2.1.3, and CALDB, version 2.7, according to recipes described in CIAO 2.1.3 threads.8 The RXTE PCA data were reduced using methods described in Weaver, Krolik, & Pier (1998), except that a later version of the spectral response matrix (version 7.10) was used. A complete description of the RXTE observation and data reduction is given in Yaqoob et al. (2002) and will not be discussed further here.

For Chandra, the instrument used in the focal plane of the High Resolution Mirror Assembly was the High Energy Transmission Grating Spectrometer (HETGS; Markert et al. 1994). The HETGS consists of two grating assemblies, a high-energy grating (HEG) and a medium-energy grating (MEG). The approximate bandpasses of the HEG and MEG are ~0.8–10 keV and ~0.5–10 keV, respectively, although the usable portion of these depends on the flux of the source. Events dispersed by the gratings are collected by a CCD array and can be assigned an energy based on the position along the dispersion axis. Since the CCDs have intrinsic energy resolution, background events can be rejected with a high efficiency, and different spectral orders can be easily discriminated. Genuine photon events collected by the CCDs fall into specific pixel patterns classified by their grade, and we retained only grades 0, 2, 3, 4, and 6. We utilized only the first-order grating data since the zeroth-order data are piled up and the higher orders carry many fewer counts than the first orders. Therefore, only the summed, negative and positive, first-order Chandra grating spectra were used in our analysis. The mean Chandra total HEG and MEG count rates were 0.2134 ± 0.0015 and 0.4813 ± 0.0022 counts s$^{-1}$, respectively. We accumulated separate HEG and MEG grating spectra from events along the dispersion direction and within ~3/6 of the peak in the cross-dispersion direction. The source flux showed little variability over the entire duration of the campaign. For example, for HEG plus MEG light curves binned at 1024 s, the excess variance above the expectation for Poisson noise (e.g., see Turner et al. 1999) was $(-0.8 \pm 3.7) \times 10^{-4}$, consistent with zero. HEG, MEG, and PCA spectra were therefore extracted over the entire on-time for each instrument. This resulted in net exposure times of 57,950 s for HEG and MEG (which includes a dead-time factor of 0.0129081) and 80,624 s for the PCA.

We made effective area files (ARFs, or ancillary response files) using CIAO 2.1.3, which also take account of the dithering of the satellite. Photon spectra (summed over the ±1 orders) were made by correcting the count spectra for the effective area and cosmological redshift but not Galactic absorption. We also extracted count spectra in a form suitable for use by the spectral-fitting package XSPEC (version 11.0.1).9 Again, we used first-order events only, combining

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7 We use $H_0 = 70$ km s$^{-1}$ Mpc$^{-1}$ and $q_0 = 0$ throughout this paper, unless otherwise stated.

8 See http://asc.harvard.edu/ciao2.1/documents_threads.html.

9 See http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec.
the positive and negative orders but keeping the HEG and MEG spectra separate for independent analysis. The spectra were produced with a range of different bin sizes, from 0.005 to 0.32 Å. The smaller bin sizes are appropriate for studying narrow spectral features that may be unresolved, and the larger bin sizes are better for studying broad features and the continuum. For reference, FWHM spectral resolutions of the HEG and MEG are 0.012 and 0.023 Å, respectively. Since the MEG soft X-ray response is much better than the HEG (whose bandpass extends down to only \( \sim 0.8 \) keV), we use the MEG as the primary instrument but refer to the HEG for confirmation of features in the overlapping bandpass and for constraining the continuum. The MEG spectral resolution corresponds to FWHM velocities of \( \sim 250, 560, \) and \( 3560 \) km s\(^{-1}\) at observed energies of 0.5, 1.0, and 6.4 keV, respectively. The HEG spectral resolution corresponds to velocities of half of these values. The response matrices “acismeg1D1999-07-22rmfN0004.fits” and “acisheg1D1999-07-22rmfN0004.fits,” combined with the ARF files described above, were used to fold models through the instrument response and thereby directly compare predicted and observed count spectra.

We did not subtract detector or X-ray background since it is such a small fraction of the observed counts (<0.5% for the MEG). We treated the statistical errors on both the photon and count spectra with particular care since the lowest and highest energies of interest can be in the Poisson regime, with spectral bins often containing a few, or even zero, counts. We assign a statistical error of \( 1.0 + (N + 0.75)^{1/2} / C_0 \) on the number of photons, \( N \), in a given spectral bin. This prescription, from Gehrels (1986), is a good approximation to the positive error for a Poissonian distribution, being good to better than 1.5% for all \( N \), but overestimates the negative error for small \( N \). As \( N \) increases, the approximation tends to the Gaussian limit. It is important to bear in mind, however, that even for 100 counts bin\(^{-1}\), \( \sqrt{N} \) still gives a statistical error that is \( \sim 10\% \) too small (the corresponding error on the approximation at this \( N \) is less than 0.1%; see Gehrels 1986). We were also careful not to propagate statistical errors when combining spectral orders or binning spectra. Statistical errors were always computed on numbers of photons in final bins, according to the above prescription, since the standard method of propagation of errors is correct only when the errors are Gaussian.

For the HEG data, the signal-to-noise ratio (SNR) per 0.02 Å bin is greater than 1 blueward of \( \sim 14 \) Å and as high as \( \sim 7 \) in the \( \sim 2-3.5 \) Å range. For the MEG data, in the \( \sim 2-25 \) Å band that we examine here, the SNR per 0.02 Å bin ranged from \( \sim 1 \) at \( \sim 20 \) Å to a maximum of \( \sim 12 \) at \( \sim 7 \) Å. The systematic uncertainty in the energy scale is currently believed to be 0.0028 and 0.0055 Å for the HEG and MEG, respectively.\(^{10}\) For the MEG, at 0.5, 1, and 6.4 keV this corresponds to velocity offsets of \( \sim 67, 133, \) and 852 km s\(^{-1}\), respectively, and about half of these values for the HEG.

3. OVERALL SPECTRUM AND PRELIMINARY SPECTRAL FITTING

We used XSPEC version 11.0.1 for spectral fitting to the HEG and MEG spectra in the 0.8–5 keV and 0.5–5 keV bands, respectively. These energy bands will be used in all the spectral fitting in the present paper, in which we concentrate on features in the soft X-ray spectrum (less than \( \sim 2 \) keV). We used the \( C \)-statistic for finding the best-fitting model parameters and quote 90% confidence, one-parameter statistical errors unless otherwise stated. The harder spectrum, out to 19 keV (using simultaneous RXTE data in addition to the Chandra data), has been discussed at length in Yaqoob et al. (2002). The hard X-ray continuum measured by Chandra MEG and HEG and RXTE was found to be well described with a single power law in the range 2–19 keV, with no Compton-reflection continuum required, and a photon index of \( \Gamma = 1.674^{+0.008}_{-0.009} \) measured from the joint three-instrument spectral fits. In all the spectral fits in the present paper, we include this hard power law component for the continuum, with \( \Gamma \) fixed at 1.674. Detailed analysis of the Fe K emission complex was also presented by Yaqoob et al. (2002), so we do not discuss this part of the spectrum further. Since we convolve all models through the instrument response before comparing with the data, all our model line widths are intrinsic values and do not need to be corrected for the instrument broadening. This contrasts with the analysis method in some of the literature on HETGS results in which models are fitted directly to the data and then corrected for instrument broadening (e.g., Kaspi et al. 2000, 2002).

First, we show how the 0.5–5 keV MEG data compare to a simple model consisting only of the hard (\( \Gamma = 1.674 \)) power law and Galactic absorption. For the latter, we use a value of \( 4.44 \times 10^{20} \) cm\(^{-2}\) (Murphy et al. 1996) throughout this work. Figure 1a shows the MEG photon spectrum of Mrk 509 binned at 0.32 Å with the model

![Figure 1](http://space.mit.edu/CXC/calib/hetecal.html)

**Fig. 1.—**Comparison of the Mrk 509 MEG spectrum to the best-fitting power-law model fitted to the 2–19 keV (joint HETGS/RXTE data) extrapolated down to 0.5 keV. Galactic absorption of \( 4.44 \times 10^{20} \) cm\(^{-2}\) is included in the model, and the power-law index is \( \Gamma = 1.674 \). The MEG data are binned at 0.32 Å. Panel (a) shows the photon spectrum, and (b) shows the ratio of the MEG data to the above model. Both panels show that the intrinsic spectrum is required to steepen at low energies, relative to the hard X-ray power law.
overlaid. The bottom panel (Fig. 1b) shows the ratio of the data to this model. This simple power law is clearly a poor fit to the data, with considerable complexity apparent, both in the continuum and in terms of discrete absorption lines and possible edges. Figure 1 clearly shows a soft X-ray excess, rising up from the hard power law (modified by Galactic absorption), below \(0.7\) keV, reaching \(\sim 60\%\) above the extrapolated hard power law spectrum. We caution that there may still be broad residual uncertainties of \(\sim 30\%\) or more in the calibration of the MEG effective area at the lowest energies.\(^{11}\) To quantitatively examine Chandra HETGS data for 3C 120 (observed in 2001 December; details will be reported elsewhere). The residuals when the MEG data are fitted with a power law plus Galactic absorption are less than \(20\%\) in the entire 0.5–5 keV band. This strongly suggests that at least part of the soft excess in Mrk 509 is real. This soft excess has been observed during simultaneous ROSAT/Ginga observations (Pounds et al. 1994), a BeppoSAX observation (Perola et al. 2000), and a recent XMM-Newton observation (Pounds et al. 2001). Both the BeppoSAX and XMM-Newton observations required a photoionized absorber as well as a soft excess. A 1994 ASCA observation, on the other hand, did not require a soft excess in addition to the complex absorber (Reynolds 1997; George et al. 1998).

The origin of the soft excess is unclear. It may be the tail end of some kind of soft thermal emission (or Comptonized soft thermal emission), possibly from an accretion disk (e.g., see Piro, Matt, & Ricci 1997 and references therein). Any relativistically broadened O vii Ly\(\alpha\) (\(\lambda 18.969\) emission) that is present could also contribute to the soft excess (e.g., Branduardi-Raymont et al. 2001; Turner et al. 2001). Since the soft excess appears only in the 0.5–1 keV band of our data, we do not have enough information to constrain its origin, and sophisticated modeling of it is not warranted. Therefore, in the remainder of this paper we model the 0.5–5 keV intrinsic continuum with a broken power law in which the hard photon index, \(\Gamma_1\), above a break energy, \(E_B\), is always fixed at 1.674 and the soft photon index, \(\Gamma_2\) (below \(E_B\)), is a free parameter, as is \(E_B\). When the data are modeled with this continuum, there is still considerable structure in the soft X-ray spectrum, indicative of the presence of a photoionized, or “warm,” absorber. Now, the warm absorber in Mrk 509 and other AGNs when observed with CCDs (such as those on ASCA) has often been modeled simply with absorption edges due to O vii and O viii since the lower CCD spectral resolution did not usually warrant more sophisticated models.

In order to directly compare the new Chandra data with previous observations, we modeled the MEG data with two absorption edges and the intrinsic continuum described above. The energies and optical depths (at threshold) of the two absorption edges were allowed to float. The best-fitting model overlaid on the MEG photon spectrum is shown in Figure 2. The best-fitting parameters obtained from this model were \(0.732^{+0.004}_{-0.003}\) and \(0.871^{+0.004}_{-0.003}\) keV for the threshold energies of O vii and O viii, respectively. For the optical depths at threshold, we obtained \(\tau = 0.30^{+0.04}_{-0.03}\) and \(0.14^{+0.05}_{-0.03}\) for O vii and O viii, respectively. All quantities refer to the rest frame of Mrk 509. The best-fitting soft X-ray photon index was 2.06, and the break energy was 1.28 keV. The measured edge energies are in good agreement with the expected values (0.739 and 0.871 keV for O vii and O viii, respectively), although the O vii edge is marginally inconsistent at a confidence level of 90% or greater. We can compare the threshold optical depths with those measured from the 1994 ASCA observation (Reynolds 1997): \(0.11^{+0.03}_{-0.02}\) (O vii) and \(0.04^{+0.04}_{-0.04}\) (O viii). The MEG values are larger (although they are consistent with lower SNR measurements from BeppoSAX data [Perola et al. 2000], which have much lower spectral resolution). However, it is known that the apparent optical depths of the O vii and O viii edges are variable in some AGNs (e.g., Otani et al. 1996; Guainazzi et al. 1996). Also, since the spectrum is so complex around the regions of the O vii and O viii edges, optical depths derived from simple models should be interpreted with caution. We show in §5 that photoionization models can adequately describe the data with smaller values of the O vii and O viii edge depths.

Even the heavily binned spectrum in Figure 2 shows a discrete feature at 0.922 keV (rest frame) corresponding to Ne ix resonance absorption. This causes the O vii edge to be somewhat deeper than that which would be obtained if the Ne ix resonance absorption were not present. Additionally, Fe M-shell unresolved transition arrays (UTAs), which have been observed in Mrk 509 and some other sources (e.g., Pounds et al. 2001; Sako et al. 2001b; Lee et al. 2001; Kaspi et al. 2002; Kaastra et al. 2002), may at some level affect the inferred column densities of both O vii and O viii.

\(^{11}\) See footnote 10.
These factors that affect the apparent O\textsuperscript{vii} and O\textsuperscript{viii} edge depths obtained from simple modeling clearly have an impact on the puzzling results from variability studies. For example, Otani et al. (1996) found that in the Seyfert 1 galaxy MCG -6-30-15, the O\textsuperscript{viii} edge depth varied (in response to the continuum) while the O\textsuperscript{vii} edge depth remained constant. In contrast, Guainazzi et al. (1996) found that the O\textsuperscript{vii} edge was variable while the O\textsuperscript{viii} edge depth remained constant. For MCG -6-30-15, Morales, Fabian, & Reynolds (2000) proposed a solution consisting of multiple, spatially separated zones to explain these results. The higher spectral resolution \textit{Chandra} data show that these issues need to be revisited. Indeed, as has been pointed out by Lee et al. (2001), more recent \textit{Chandra} observations of MCG -6-30-15 suggest that the O\textsuperscript{viii} edge in this source is complicated by Ne\textsubscript{x}ix resonance absorption, as well as a complex of lines from Fe\textsubscript{xvii} and Fe\textsubscript{xviii}.

4. SPECTRAL FEATURES AND KINEMATICS

4.1. Absorption and Emission Lines

In order to best illustrate different characteristics of the spectrum, we display the spectral data in several different ways. In Figure 3 we show the MEG photon spectrum below \~1.4 keV, as a function of observed energy, along with the deduced intrinsic broken power law continuum (not corrected for Galactic absorption), as derived from the best-fitting photoionization model described in § 5. The solid red curve in Figure 3 is the photoionization model itself (the details of which are deferred to § 5). The data and the models in Figure 3 are all absorbed by the Galactic column density. An important point to realize from Figure 3 is that in some regions the spectrum is so complex that it is difficult to distinguish absorption from emission. For example, at observed energies between \~0.7 and 0.8 keV, there appears to be a complex emission feature relative to the continuum.

![Figure 3](image.png)

Fig. 3.—Mrk 509 MEG observed photon spectrum compared to the best-fitting photoionized absorber model (red solid line). Also shown is the intrinsic continuum (blue solid line) modified by Galactic absorption (neither the data nor model have been corrected for Galactic absorption). The dashed lines show the expected positions of some bound-free absorption edges. The model consists of an intrinsic continuum, which is a broken power law (best-fitting break energy at 1.04 keV), absorbed by photoionized gas with best-fitting ionization parameter of log ζ = 1.76 (or log U = 0.27) and column density 2.06 × 10\textsuperscript{21} cm\textsuperscript{-2}. Full details of the model calculations, fitting procedures, and discussion of the details of the comparison between data and model can be found in § 5. The 0.7–0.9 keV region is very complex, so simple two-edge models fitted to older CCD data (of Seyfert 1 galaxies in general) could have been biased by this complexity. In particular, note that the apparent emission feature at \~0.78–0.79 keV (observed) is consistent with unabsorbed continuum and strong absorption on either side. There is also an instrumental feature at \~0.8 keV that may partly be responsible for the poor fit in this region. The panel showing the Mg\textsubscript{xi}(r) 1s\textsuperscript{2}–1s2p (λ9.169) line, with data binned at 0.02 Å, is shown separately for clarity, since there are no significant features between the end of the previous panel (at 1.15 keV) and the Mg\textsubscript{xi}(r) 1s\textsuperscript{2}–1s2p (λ9.169) absorption line. The remaining data above 0.5 keV are binned at 0.08 and at 0.04 Å below 0.5 keV.
local two-edge model continuum in Figure 2, but from Figure 3 it is clear that the peak flux of this feature (between \( \sim 0.78 \) and \( 0.79 \) keV, observed) coincides with the inferred intrinsic continuum, implying that the apparent feature is simply due to the presence of broad absorption complexes on either side of it. Also, there is a sharp variation in the MEG effective area at \( \sim 0.8 \) keV, and any uncertainties here could manifest themselves as apparent spectral features (see § 5 for further discussion).

In Figures 4 and 5, we show the MEG and HEG spectra, respectively, this time as a function of wavelength in the source rest frame, redward of 2 Å. These spectra have a bin size of 0.02 Å, approximately the FWHM MEG spectral resolution (0.023 Å). Below each panel showing the data, the SNR in each bin, so that one can easily gauge the statistical significance of any spectral features. The same MEG data are also displayed in Figures 6 and 7. In Figure 6 we overlay the Lyman series (blue) for H-like N, O, Ne, Mg, Si, S, and Ar and the corresponding He-like triplets (red) that lie in the 2–25 Å range. In Figure 7 we overlay the He-like resonance series lines (blue) to the \( n = 1 \) level for the same elements and, in addition, the Balmer lines (red) of the hydrogenic ions of Si, S, and Ar.

Referring to Figures 3–7, we see that the strongest, clear discrete spectral features detected are absorption lines due to Ne \( \text{vii} \) Ly\( \alpha \) (\( \lambda 24.781 \)), N \( \text{vii} \) Ly\( \beta \) (\( \lambda 20.910 \)), O \( \text{viii} \) Ly\( \alpha \) (\( \lambda 18.969 \)), Ne \( \text{ix} \) (\( \lambda 13.447 \)), Ne \( \text{ix} \) (\( \lambda 15.149 \)), Ne \( \text{ix} \) (\( \lambda 12.134 \)), and Mg \( \text{xi} \) (\( \lambda 9.169 \)). Some strong Fe absorption lines are also detected. Weaker absorption lines are also apparent from the spectra, such as higher order Lyman lines of O and Ne (there is evidence for transitions up to \( n = 5 \) in each case). Higher SNR X-ray spectroscopy of NGC 3783 (Kaspi et al. 2002) has shown that blending of absorption features considerably complicates the spectrum. In particular, lines from Fe \( \text{xvii} \), Fe \( \text{xix} \), and Fe \( \text{x} \) \( \text{xxi} \) are likely to be blended with the absorption troughs at \( \sim 11.5 \), 12.1, 13.4, and 16.0 Å in the Mrk 509 spectrum. We note that we do not detect absorption from the highest ionization states of elements beyond Ne, such as Si \( \text{xiv} \) Ly\( \alpha \) (\( \lambda 0.182 \); see Fig. 6). Thus, the ionization state of the absorber cannot be so high that Si \( \text{xiv} \) is abundant.

Apart from Fe K\( \alpha \) and some tentative emission features at \( \sim 9.3, 9.6, 9.8, \) and 12.6 Å (possibly attributable to Fe \( \text{x} \) \( \text{xx} \)), no other emission-line features are clearly identifiable. In particular, we do not detect the O \( \text{viii} \) He-like triplet, which was detected during an X\( \text{MM-Newton} \) observation, by Pounds et al. (2001). In § 6 we shall give a more detailed comparison with the X\( \text{MM-Newton} \) observation.

The presence of broad, bound-free absorption features and many narrow features that may be blended makes it impossible to define an observed continuum for much of the spectrum and therefore difficult to measure meaningful equivalent widths (EWs) of even the strongest narrow absorption features. Rather than try to measure equivalent widths of all candidate features and compare with model predictions, we take the physically more direct approach of fitting photoionization models to the data (§ 5). Nevertheless, in the process of measuring the observed energies of the strongest discrete absorption features, we did attempt to measure the equivalent widths of some absorption lines. The measurements were made using the broken power law plus two-edge model as the baseline spectral model (see § 3) and Gaussians to model the absorption lines. The continuum and edge parameters were frozen at the best-fitting values given in § 3, and the data were fitted over a few hundred eV centered on the feature of interest. The fitted range of the data was extended down to 0.47 keV in order to measure the parameters of N \( \text{vii} \) Ly\( \alpha \) (\( \lambda 24.781 \)). Initially, the intrinsic width of each Gaussian was frozen at less than the instrumental resolution, but it was then allowed to float in order to investigate whether the lines were resolved. The results for the measured energies, apparent velocity shifts relative to systemic, equivalent widths, and intrinsic widths of these strongest absorption features are given in Table 1. Note that the quoted equivalent widths are relative to the intrinsic continuum. Again, we caution that the measured equivalent widths have been rounded to the nearest 5 km s\(^{-1}\).

### Table 1

| Line\( ^{a} \) | EW (Data)\(^{b} \) (eV) | EW (Model)\(^{b} \) (eV) | Velocity\(^{d} \) (km s\(^{-1}\)) | FWHM (km s\(^{-1}\)) |
|---|---|---|---|---|
| N \( \text{vii} \) Ly\( \alpha \) (\( \lambda 24.781 \)) | 0.55\(^{0.15} \)\(^{e} \) | 0.33 | 100 | <310 |
| N \( \text{vii} \) Ly\( \beta \) (\( \lambda 20.910 \)) | 0.64\(^{0.26} \)\(^{e} \) | 0.67 | 320 | <320 |
| O \( \text{viii} \) Ly\( \alpha \) (\( \lambda 18.969 \)) | 0.72\(^{0.18} \)\(^{e} \) | 0.94 | 250 | <450 |
| Ne \( \text{ix} \) (\( \lambda 13.447 \)) | 1.33\(^{0.30} \)\(^{e} \) | 1.08 | 220 | 440–590 |
| Ne \( \text{ix} \) (\( \lambda 15.149 \)) | 1.12\(^{0.20} \)\(^{e} \) | 0.87 | 180 | <890 |
| Mg \( \text{x} \) (\( \lambda 9.169 \)) | 0.68\(^{0.20} \)\(^{e} \) | 1.05 | 620 | 1040 |
| Ne \( \text{x} \) Ly\( \alpha \) (\( \lambda 12.134 \)) | 1.89\(^{0.37} \)\(^{e} \) | 0.96 | 210 | 875–550 |
| Ne \( \text{x} \) Ly\( \alpha \) (\( \lambda 12.134 \)) | 1.08\(^{0.39} \)\(^{e} \) | 0.96 | 355 | 1 (fixed) |

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\(^{a}\) Laboratory-frame wavelengths.

\(^{b}\) Measured equivalent widths in the Mrk 509 frame.

\(^{c}\) Predicted equivalent widths using \( b = 100 \) km s\(^{-1}\) and XSTAR columns (§ 5.4).

\(^{d}\) Velocity offset (Mrk 509 frame) of Gaussian centroid relative to systemic. Negative values are blueshifts.

\(^{e}\) No meaningful upper limits because of poor statistics and line saturation.

\(^{f}\) Different centroids were obtained for Ne \( \text{x} \) Ly\( \alpha \) (\( \lambda 12.134 \)) depending on whether the intrinsic width of the Gaussian was fixed at 1 km s\(^{-1}\) or a free parameter, indicating a complex profile (see § 4 and Fig. 8).
Fig. 4.—*Chandra* MEG photon spectrum for Mrk 509 against wavelength in the source rest-frame (binned at 0.02 Å, approximately the MEG FWHM spectral resolution). The corresponding SNR per bin is also shown. The spectrum has not been corrected for Galactic absorption. Many discrete absorption features are identifiable, but none are labeled in this plot since it is primarily for finding the SNR at a particular wavelength. The same spectrum is shown in Figs. 6 and 7, but this time with labels corresponding to different arrays of atomic transitions. See also Fig. 3, which shows the ~0.47–1.4 keV region of the spectrum with some important atomic features labeled.
widths are subject to uncertainties in the continuum, line blending, and any complexity in the line profile. It is instructive to compare line strengths with a physical model, so also given in Table 1 are the predicted equivalent widths from the best-fitting photoionization model discussed in §5.

4.2. Absorption-Line Velocity Profiles

Table 1 shows that all of the measured absorption lines are blueshifted, with Gaussian-fitted centroids ranging from near systemic velocity to \( \sim -600 \) km s\(^{-1}\). However, some of the velocity profiles appear to be more complex than Gaussian, as can be seen from Figure 8 (which shows the profiles of Ne x Ly\( \alpha \) [\( \lambda 12.134 \)], Ne ix [r] 1s\(^2\)-1s2p [\( \lambda 13.447 \)], Mg xi [r] 1s\(^2\)-1s2p [\( \lambda 9.169 \)], and O viii Ly\( \alpha \) [\( \lambda 18.969 \)])). They are centered with zero at the systemic velocity of Mrk 509, with positive and negative velocities corresponding to redshifts and blueshifts, respectively. The velocity profiles were obtained from combined HEG and MEG data except for the O viii Ly\( \alpha \) [\( \lambda 18.969 \)] profile, which was determined using MEG data only, since at this energy the HEG effective area is negligible. It can be seen from Table 1 and Figure 8 that the velocity offset for all of the absorption lines is consistent with \( \sim -200 \) km s\(^{-1}\), except for the Mg xi (r) resonance line. The latter has an apparent minimum at \( \sim -600 \) km s\(^{-1}\), which may indicate a truly different absorption-line profile, or the different offset velocity may be an artifact of contamination from other absorption lines, or there may be emission filling in a trough at \( \sim -200 \) km s\(^{-1}\).

Table 1 also shows that the Ne x Ly\( \alpha \) (\( \lambda 12.134 \)) and Ne ix 1s\(^2\)-1s2p (\( \lambda 13.447 \)) lines appear to be marginally resolved, while all the other lines are unresolved (FWHM < 300 km s\(^{-1}\) for the lightest elements, going up to FWHM < 1030 km s\(^{-1}\) for Mg). The Ne x Ly\( \alpha \) (\( \lambda 12.134 \)) line is particularly interesting because we obtain a different centroid offset velocity depending on whether the Gaussian model has an intrinsic width fixed at a value much less than the instrument resolution, or whether the intrinsic width is a free parameter. The latter gives a marginally better fit (\( \Delta \chi^2 = -4.0 \)), with an offset of \( \sim -210 \) km s\(^{-1}\), and a broad line, but still with FWHM < 1300 km s\(^{-1}\). The narrow-line fit gives a higher blueshift, but in both cases the lower limit on the velocity offset is the same, at \( \sim -400 \) km s\(^{-1}\). This is
Fig. 6.—*Chandra* MEG photon spectrum for Mrk 509 against wavelength in the source rest frame (binned at 0.02 Å, approximately the MEG FWHM spectral resolution). Labels show the Lyman series wavelengths (blue) for Ar, S, Si, Mg, Na, Ne, O, and N. Also shown (red) are the wavelengths of the helium-like triplets (resonance, intercombination, and forbidden lines) of Ar, S, Si, Mg, Ne, and O.
Fig. 7.—*Chandra* MEG photon spectrum for Mrk 509 against wavelength in the source rest frame (binned at 0.02 Å, approximately the MEG FWHM spectral resolution). Plotted in blue are the wavelengths of He-like resonance-absorption transitions ($n = 1 \rightarrow 2, 3, 4, \ldots$) of Ar, Si, Mg, Na, Ne, O, and N. Also shown (red) are the Balmer series transitions of Ar, S, and Si.
The absorption features lie at around \(\lambda_{C0}\) and the principal seven kinematic components of the UV absorber are also compared with the FWHM MEG velocity resolution of 352, 496, 550, and \(472 \text{ km s}^{-1}\) for O viii Ly\(\alpha\) (189.669), Ne ix (r) 1s\(^2\)-1s2p (134.447), Ne x Ly\(\alpha\) (121.34), and Mg x (r) 1s\(^2\)-1s2p (9.169), respectively. The velocities of these seven kinematic components of the UV absorber are also shown (blue) and are -422, -328, -259, -62, -22, +34, and +124 \(\text{ km s}^{-1}\) (see Paper II).

indicative of a complex velocity profile. However, the MEG FWHM velocity resolution goes from \(\sim 280 \text{ km s}^{-1}\) for the lowest energy transitions (nitrogen lines), up to \(\sim 730 \text{ km s}^{-1}\) for the highest energy transition (Mg xi [r]), so any apparent structure in the profiles should be interpreted with caution. The resolution at Ne x Ly\(\alpha\) (121.34) is 550 \(\text{ km s}^{-1}\), FWHM. The complexity in the velocity profiles, if real, may either be intrinsic or due to contamination from other absorption and/or emission features. The intrinsic complexity could be due, for example, to the presence of several kinematic components, making different contributions to the overall profile, as is the case for UV lines (see § 7).

Figure 8a shows that the broad trough in the Ne x Ly\(\alpha\) (121.34) profile, centered at \(\sim -200 \text{ km s}^{-1}\), extends redward of the systemic velocity, perhaps by up to \(\sim +400 \text{ km s}^{-1}\). Figure 8b is centered around the Ne ix (r) 1s\(^2\)-1s2p (134.447) transition, and the velocity profile appears to be much more asymmetric than Ne x Ly\(\alpha\) (121.34), having a clear, single minimum at \(\sim -200 \text{ km s}^{-1}\). The profile of Ne ix (r; \(\lambda_{134.447}\)) appears to be just as broad as Ne x Ly\(\alpha\) (121.34); however, Figure 8c shows the velocity profile for Mg xi (r) 1s\(^2\)-1s2p (9.169), which appears to have two minima, one at \(\sim -600 \text{ km s}^{-1}\) and the other at systemic. It is possible that the profile is really the same as that of Ne ix (r; \(\lambda_{134.447}\)), with the trough contaminated by emission. The velocity profile of O viii Ly\(\alpha\) (189.669) shown in Figure 8d is very similar to that of Mg xi (r; \(\lambda_{9.169}\)), with two minima at the same velocities, except that the contrast of the minima with the center of the profile is not so high.

Figure 9 shows velocity spectra centered on several atomic transitions that are not significantly detected in the data (Na xi Ly\(\alpha\) (\(\lambda_{10.025}\)), Ar xviii Ly\(\alpha\) (\(\lambda_{3.733}\)), Mg xi Ly\(\alpha\) (\(\lambda_{8.421}\)), and Si xiv Ly\(\alpha\) (\(\lambda_{6.182}\))). The abundances of Na and Ar are small compared to oxygen and neon, for example, partially accounting for the absence of features due to these ions. There is a hint of Mg xi Ly\(\alpha\) (\(\lambda_{8.421}\)) absorption, but it is very weak if present. Si xiv Ly\(\alpha\) (\(\lambda_{6.182}\)) is clearly not present in absorption in the data, although there is a hint of emission. Since the cosmic abundances of silicon and magnesium are similar and since we see Mg xi (r) but we do not see Si xiv Ly\(\alpha\) (\(\lambda_{6.182}\)), this constrains the ionization state of the absorber and will therefore be important for photoionization modeling, discussed in § 5.
The velocity profiles in Figure 8 are reminiscent of *Chandra* observations of absorption features in other AGNs. The absorption is generally blueshifted with respect to the systemic velocity, and there is evidence of multiple kinematic components and multiple ionization states (e.g., NGC 4051, Collinge et al. 2001; NGC 3783, Kaspi et al. 2002; NGC 5548, Kaastra et al. 2002, T. Yaqoob, B. McKernan, I. M. George, & T. J. Turner 2003, in preparation). Because of the limited spectral resolution of *Chandra*, it is possible that there are actually many unresolved kinematic components making up the velocity profiles, and we shall return to this point in §7, where we examine the relationship between the X-ray and UV absorbers.

5. PHOTOIONIZATION MODELING

We used the photoionization code XSTAR, version 2.1.d, to generate several grids of models of emission and absorption from photoionized gas in order to directly compare with the data. In Paper II, CLOUDY is used to model the UV data. We use the default solar abundances in XSTAR and CLOUDY. For reference, these abundances are given in Table 2.

5.1. The Spectral Energy Distribution

First, we constructed a spectral energy distribution (SED) for Mrk 509 as follows. Average radio and infrared fluxes were obtained from Ward et al. (1987). UV fluxes were obtained from our *HST/STIS* spectrum, observed simultaneously with *Chandra*, from continuum regions centered on 1181, 1366, 1510, 2291, and 3013 Å (observed frame). The fluxes were dereddened using the Galactic reddening curve of Savage & Mathis (1979) and a reddening value of $E(B-V) = 0.08$, corresponding to the observed H I Galactic column (Shull & Van Steenberg 1985). Further details of the UV data analysis can be found in Paper II. In principle, the X-ray portion of the SED must be derived iteratively because the intrinsic X-ray continuum can be deduced only from fitting the data self-consistently with a model of the absorption (which is complex and affects the X-ray data over a broad energy range, up to nearly 2 keV).

In practice, we implemented a two-step process to obtain a fiducial SED and then investigated the effects of adjusting this SED in a manner described below. For the first of the two steps, we started with an SED in which the X-ray spectrum was a single power law with a photon index of 1.674 (consistent with *Chandra/RXTE* data above 2 keV; see Yaqoob et al. 2002), extrapolated down to 0.5 keV. The 0.5 keV point was then simply joined onto the last UV point by a straight line in log-log space (this corresponds to a slope of $-1.44$ in $L_\nu$ vs. $\nu$). The hard X-ray power law in this and subsequent SEDs extended out to 500 keV. Grids of photoionization models (details of which are given below) were then generated using this initial SED, and the *Chandra* MEG and HEG data were then fitted below 5 keV using a broken power law model for the intrinsic continuum, modified by the photoionized absorber and Galactic absorption. The hard power law index was kept fixed at $\Gamma_1 = 1.674$. We obtained a soft power law index of $\Gamma_2 = 2.19$ and a break energy of 1.05 keV. In the second step, we used the broken power law, with the above parameters (and normalization obtained from the spectral fit), for the X-ray portion of the SED, down to 0.5 keV. Again, we connected the 0.5 keV point to the last UV point by a straight line in log-log space. The resulting SED is shown in Figure 10 (filled circles connected by solid lines). The dashed curves show variations on this SED, constructed by raising and lowering the flux at 55 eV (the energy required to doubly ionize He) by a factor of 1.5. These latter two SEDs will be used to investigate the effects of uncertainties in the unobserved part of the SED by comparing with the results obtained with the baseline SED. Also shown in Figure 10 is the "mean AGN" SED derived by Matthews & Ferland (1987).

5.2. Model Grids

The photoionization model grids used here are two-dimensional, corresponding to a range in values of equiva-

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**TABLE 2**

| Element | Abundance |
|---------|-----------|
| H       | $1.00 \times 10^0$ |
| He      | $1.00 \times 10^{-1}$ |
| C       | $3.54 \times 10^{-4}$ |
| N       | $9.33 \times 10^{-5}$ |
| O       | $7.41 \times 10^{-4}$ |
| Ne      | $1.20 \times 10^{-4}$ |
| Mg      | $3.80 \times 10^{-5}$ |
| Si      | $3.55 \times 10^{-5}$ |
| S       | $2.14 \times 10^{-5}$ |
| Ar      | $3.31 \times 10^{-6}$ |
| Ca      | $2.29 \times 10^{-6}$ |
| Fe      | $3.16 \times 10^{-6}$ |
| Ni      | $1.78 \times 10^{-6}$ |

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**Fig. 10.**—Observed and interpolated baseline SED (solid curve) used for photoionization modeling of Mrk 509. Average radio and IR fluxes are from Ward et al. (1987). The UV data are dereddened fluxes from the *HST/STIS* observation (Kraemer et al. 2003), and the X-ray data points are from our simultaneous *Chandra* HETGS data. The hard X-ray power law has $\Gamma = 1.674$ and has been extended to 500 keV. The dashed lines are deviations representing modifications to the baseline SED used to investigate the effects of uncertainties in the unobserved part of the SED. The modifications to the baseline SED correspond to changing the flux at 55 eV (just above the ionization energy of neutral He) by ±50%. See §5.1 for full details of the construction and applications of the SEDs. The dotted curve is the "mean AGN" SED of Matthews & Ferland (1987), normalized to the same ionizing luminosity (i.e., in the range 1–1000 ryd) as that of the Mrk 509 baseline SED.
lent neutral hydrogen column density, \(N_{\text{H}}\), and the ionization parameter, \(\xi = L_{\text{ion}}/(n_e r^2)\) ergs cm\(^{-1}\) s\(^{-1}\). Here \(L_{\text{ion}}\) is the ionizing luminosity (in ergs s\(^{-1}\)), in the range 1–1000 ryd, \(n_e\) is the electron density in cm\(^{-3}\), and \(r\) is the distance of the illuminated gas from the ionizing source in centimeters.\(^{12}\)

The grids were computed for equipursed intervals in the logarithms of \(N_{\text{H}}\) and \(\xi\), which ranged from \(5 \times 10^{20}\) to \(5 \times 10^{23}\) cm\(^{-2}\) and 0.5–2.5, respectively. The X-ray data cannot constrain the electron density since we do not detect any suitable emission lines, so we fixed \(n_e\) at \(10^6\) cm\(^{-3}\) in most of the grids. For diagnostic purposes, some grids were constructed with \(n_e\) as low as \(10^2\) cm\(^{-3}\) and as high as \(10^{11}\) cm\(^{-3}\). We confirmed that results from fitting the photoionized absorber models to the X-ray data were indistinguishable for densities in the range \(n_e = 10^2–10^{11}\) cm\(^{-3}\). Hereafter, all XSTAR models discussed correspond to a density of \(10^8\) cm\(^{-3}\), unless otherwise stated. This value is arbitrary and does not signify any preference for high densities.

Finally, all models assumed a velocity turbulence \((b\)-value\) of 1 km s\(^{-1}\), and since XSTAR broadens lines by the greater of the turbulent velocity and the thermal velocity, it is the latter which is relevant for these models. As the turbulent velocity increases, the equivalent width of an absorption line increases for a given column density of an ion. Therefore, to calculate model equivalent widths correctly, one must know what the velocity width is (note that the \(b\)-value could represent all sources of line broadening). We cannot simply extend the XSTAR model grids into another dimension (velocity width) and deduce a \(b\)-value directly from model fitting, because we are limited by the finite internal energy resolution of XSTAR. The widths of the energy bins of the XSTAR model grids are in the range \(\sim 200–600\) km s\(^{-1}\). Our choice of velocity width \((b\)-value corresponding to the thermal width\) ensures that the energy resolution of XSTAR is the limiting factor and not the \(b\)-value itself. We will then need to take a rather more complicated approach to model fitting, which we describe in \S\ 5.3 below.

5.3. Model Fitting

We proceeded to fit the MEG and HEG spectra (binned at 0.08 Å) simultaneously, with all corresponding model parameters for the two instruments tied together, except for the relative normalizations. The intrinsic continuum was a broken power law (the hard photon index again fixed at 1.674) modified by absorption from photoionized gas and the Galaxy. Excluding overall normalizations, there were a total of four free parameters, namely, the column density of the warm absorber, \(N_{\text{H}}\), the ionization parameter, \(\xi\), the intrinsic soft photon index, \(\Gamma_2\), and the break energy of the broken power law continuum, \(E_B\).

Our model-fitting strategy is more complicated than simply comparing the XSTAR model spectra with the data since the XSTAR spectra assume a certain line width \((b\)-value\), which itself is limited by the finite internal energy resolution of XSTAR. We chose \(b = 1\) km s\(^{-1}\) in order that the energy resolution of XSTAR is the limiting factor. The result is that the equivalent widths of lines in the XSTAR spectra need to be calculated more rigorously using a line width \((b\)-value\) appropriate for the data. On the other hand, the ionic columns in the XSTAR models are robust from this point of view and do not depend on the velocity width. Therefore, after finding the best-fitting ionization parameter and warm-absorber column density from a global fit using the model described above, in \S\ 5.4 we will deduce a \(b\)-value from a curve-of-growth analysis, using ionic column densities from the best-fitting global model. We will then construct detailed model profiles for each of the detected absorption lines.

The best-fitting parameters derived from the XSTAR global model fits were \(N_{\text{H}} = 2.06^{+0.39}_{-0.28} \times 10^{21}\) cm\(^{-2}\) and \(\log \xi = 1.76^{+0.13}_{-0.14}\) ergs cm\(^{-1}\) s\(^{-1}\) (or \(\log U = 0.27\)). The broken power law model corresponding to this best fit had a break energy of \(E_B = 0.95^{+0.15}_{-0.09}\) keV and a soft power law photon index of \(\Gamma_1 = 2.36^{+0.21}_{-0.10}\), values that are consistent with the SED that was used as input to the models. Figure 11 shows the best-fitting model folded through the MEG response and overlaid onto the MEG counts spectrum. The lower panel of Figure 11 shows the ratio of the data to the best-fitting model. Figure 12 shows the actual best-fitting XSTAR model before folding through the instrument response. Figure 13 shows the 68%, 90%, and 99% joint confidence contours of \(\log \xi\) versus \(N_{\text{H}}\). Overall, the fit is very good, and it is already apparent that the best-fitting parameters that describe the overall spectrum also give good fits to the most prominent absorption lines and edges. This can also be seen in Figure 3, which shows the best-fitting model overlaid on the photon spectrum, and in Figures 8 and 9, which show close-ups of the data and model (in velocity space), centered on particular atomic transitions. We note that, formally, a second solution with a higher column density \((\sim 3 \times 10^{21}\) cm\(^{-2}\)) but similar ionization parameter is also viable, but the best-fitting break energy of the intrinsic continuum is at \(\sim 2.15 \pm 0.25\) keV, inconsistent with the input SED and with the measured value for the first solution. We can therefore eliminate this second solution.

The main driver of these broadband fits is the overall shape of the observed spectrum, but the narrow absorption lines and the absorption edges also affect the fits. Since the centroids of the absorption lines are blueshifted, a velocity offset had to be applied to the XSTAR model. Although the velocity offsets may be different for different absorption lines (see \S\ 4.2), the SNR of the data is such that anything more complex than a single velocity offset for all the absorption lines is not warranted. We therefore applied a nominal velocity offset of \(-200\) km s\(^{-1}\) relative to systemic, which was satisfactory for all of the absorption features. We had to apply an additional (but nonphysical) correction of \(-270\) km s\(^{-1}\). The reason for the latter offset is that the code XSTAR, version 2.1.d, contains hard-wired wavelengths of some atomic transitions that disagree with wavelengths published elsewhere.\(^{13}\) We found that a simple, single offset of \(-270\) km s\(^{-1}\) was required, and Figure 3 shows that this gives an excellent fit for all the detected absorption lines (reported in Table 1), except possibly Mg xi (\(r\) 1s\(^2\)–1s2p (\(\lambda\) 9.169)). The latter has negligible impact on the spectral fit, given the SNR of the data. The fact that the individual

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\(^{12}\) In Paper II, a different ionization parameter is used, \(U = Q_{\text{ion}}/(4\pi n_e c^2)\). Here \(Q_{\text{ion}}\) is the number of ionizing photons above 1 ryd, \(c\) is the speed of light, and \(n_e\) and \(r\) have the same meaning as for \(\xi\). From our baseline SED, the conversion factor is \(U = 0.03208 \xi\), or \(\log U = \log \xi - 1.49\). Therefore, our best-fitting value of \(\log \xi = 1.76\) corresponds to \(U = 1.85\), or \(\log U = 0.27\).

\(^{13}\) For example, in the Atomic Line List (at http://www.pa.uky.edu/~peter/atomic).
model line profiles give good fits to the data (Fig. 8) and were calculated using the ionic column densities from the best-fitting XSTAR model, published wavelengths, and the deduced $b$-value (see § 5.4) shows that the various assumptions are good for our purpose.

We mentioned in § 3 that the 2.0–2.5 keV region in the Chandra spectra suffers from systematics as large as $\sim 20\%$ in the effective area due to limitations in the calibration of the X-ray telescope absorption edges in that region. We therefore omitted the 2.0–2.5 keV regions of the Chandra spectra during the spectral fitting so that the fits would not be unduly biased. These and other instrumental absorption features can be seen in the upper panel of Figure 11. All the MEG data in the 0.5–5 keV band are shown here, although the 2.0–2.5 keV region was omitted during spectral fitting. Other regions that have sharp changes in the effective area also show notable mismatches between data and model, but these are not as bad as in the 2.0–2.5 keV region. In particular, the region between $\sim 0.76$–0.81 keV shows an apparent broad emission feature. However, the entire region in the $\sim 0.7$–0.9 keV is spectrally very complex (see Fig. 3). We also mentioned in § 4.1 that the peak of the apparent emission between 0.78–0.79 keV (observed) actually coincides with the intrinsic continuum (Fig. 3) and so could be the result of a lack of absorption rather than an emission feature. However, we see that our best-fitting XSTAR model actually predicts absorption due to O viii Ly$\gamma$ and Fe xvii (at an observed energy of $\sim 0.78$–0.79 keV, or $\sim 0.81$–0.82 keV rest frame). This implies that there must be some emission features in the data. We were not able to model this emission with the emitted spectra from the XSTAR models, even with $\xi$ and $N_H$ unconstrained (without overpredicting other features that are not observed). Note that there is also emission (above the intrinsic continuum) at 0.80 keV (0.828 keV rest frame); Fe xvii and Fe xviii lines are possible candidates. However, we should remember that the region of the spectrum around 0.8 keV does coincide with a sharp change in the MEG effective area (Fig. 11), so it is likely that the poor fit here may in part be due to calibration uncertainties. Nevertheless, we confirmed that omitting the data in the region $\sim 0.76$–0.81 keV had a negligible effect on the derived best-fitting model parameters, so we decided to retain the data in this region since the uncertainties are certainly not as large as those in the 2–2.5 keV region.

5.4. Detailed Comparison of Data and Photoionization Model

In this section we compare in detail the best-fitting XSTAR photoionized absorber model and the data (refer to

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14 See http://asc.harvard.edu/udocs/docs/POG/MPOG/node13.html.
log $U$ spectra were binned at 0.08 A, we can compare the model and data at higher spectral resolution, depending on the SNR of the feature in question. As discussed in § 4.1, the strongest absorption-line features in the Chandra data are N vii Lyα ($\lambda$24.781), N vii Lyβ (λ20.910), O viii Lyα (λ18.969), Ne ix (r) 1s$^2$-1s2p ($\lambda$13.447), Ne x Lyα (λ12.134), Ne ix (r) 1s$^2$-1s3p ($\lambda$11.547), and Mg xi (r) 1s$^2$-1s2p ($\lambda$9.169; see also Table 1). No strong, identifiable emission features were found below 5 keV. Figure 3 shows that the best-fitting XSTAR model described above ($N_H = 2.06 \times 10^{21}$ cm$^{-2}$, log $U = 1.76$ [or log $U = 0.27$]) predicts the strength of all these absorption lines very well, despite the fact that in this direct comparison the model equivalent widths have not been computed for the correct line width ($b$-value), as explained at the end of § 5.3.

In order to determine what the appropriate $b$-value might be, we calculated curves of growth for different values of $b$ (see Fig. 14). We can see from Table 1 that all the Lyα transitions from H-like and He-like ions have approximately the same measured equivalent widths, within errors. This suggests that all of these lines are on the saturated part of the curve of growth. The theoretical curves of growth in Figure 14 indicate that the measured equivalent widths of $\sim 10^{-2}$ Å are all consistent with $b \approx 100$ km s$^{-1}$. This is a rather model-independent conclusion since this deduction does not utilize any information from the XSTAR modeling. We also plotted the measured equivalent widths from Table 1 (converted to angstroms) as a function of ionic column density (from the best-fitting XSTAR model described above) and overlaid these on the curves of growth (Fig. 14). This again illustrates that, for solar abundances, all the measurements are consistent with $b = 100$ km s$^{-1}$ (except possibly O vii Lyα [\$\lambda$18.969]). The predicted equivalent widths for $b = 100$ km s$^{-1}$ are shown in Table 1 so that they can be compared directly with the observed equivalent widths.

The velocity profiles in Figure 8 (for four of the strongest absorption lines: Ne x Lyα [\$\lambda$12.134], Ne ix [r; \$\lambda$13.447], Mg xi [r; \$\lambda$9.169], and O viii Lyα [\$\lambda$18.969]) also show very good agreement between data and model. In this case the model curves were calculated using the broken power law and two-edge continuum described in § 3, a Gaussian for the absorption line, with $\sigma = b/2 = 70.7$ km s$^{-1}$, and an equivalent width from Table 1. Figure 9 illustrates that
TABLE 3
IONIC COLUMN DENSITIES

| Ion   | X-Ray (Predicted)a | UV (Predicted)b | UV (Measured)b | Ion   | X-Ray (Predicted)a |
|-------|-------------------|----------------|---------------|-------|-------------------|
| H      | 1.4 × 10^4       | 1.6 × 10^4c    | 4.7 × 10^1    | Mg vi  | 3.0 × 10^2       |
| C iv   | 3.0 × 10^-7      |                | <3.5 × 10^-1  | Mg vii | 4.9 × 10^1       |
| C iv   | 6.7 × 10^-4      | 5.5 × 10^-1   | <5.1 × 10^-4  | Si xiv | 3.8 × 10^6       |
| C iv   | 1.2 × 10^-1      | 7.3           | 7.3           | Ar xvii | 1.6 × 10^-3    |
| N v    | 8.5 × 10^-1      | 7.1           | 7.0           | Fe xx   | 8.4 × 10^6       |
| O vi   | 7.1 × 10^2       | 1.2 × 10^2    | 0.82 × 10^2   | Fe xiv  | 1.0 × 10^2       |
| O vii  | 3.5 × 10^1       |                |               | Fe xv   | 1.8 × 10^2       |
| O vii  | 8.1 × 10^0       |                |               | Fe xvii | 1.6 × 10^2      |
| Ne ix  | 1.4 × 10^1       |                |               | Fe xviii | 5.1 × 10^1     |
| Ne x   | 7.5 × 10^2       |                |               | Fe xix  | 7.6 × 10^9       |

Note.—All values in units of 10^{14} cm⁻².

a Predicted and measured UV column densities are summed over available measurements from all UV kinematic components except the low-ionization component of Fe (see Paper II). H, C iv, and O vi measurements are from Kriss et al. 2000 and not the present observations. Predicted UV column densities are from CLOUDY photoionization models of the UV data.

b Column from all kinetic components except 4 (low) and 4’ (see Paper II).

...some features not predicted by the model are indeed not detected in the data (as would be expected from the low ionization in Table 3). These include Ar xviii Lyα (λ3.733), Na xi Lyα (λ10.025), Mg xii Lyα (λ8.421), and Si xiv Lyα (λ6.182). These are all higher ionization features (and Na and Ar have relatively low abundance), so we can see that the absence of features from these ions in the data contributes to the strong constraints on the ionization parameter. Thus, our single-component photoionization model gives surprisingly good fits to the principal absorption lines.

There are many more discrete absorption features apparent in the spectra but with lower SNR. Although these individual weak features cannot be studied in detail, we can at least check whether the best-fitting XSTAR model does not conflict with the data. We found that, as far as narrow absorption lines are concerned, all absorption lines predicted by the model were consistent with the data, with the exception of the 0.78–0.79 keV (observed) region, which has already been discussed in §§ 3 and 4.1 (see Fig. 3). In particular, we found that the model agrees well with the data for the low-order Lyman transitions of Ne and O. The first five O vi 1s–np resonance lines also agree well with the data (the rest are too weak). Conversely, the data show possible absorption features that are not predicted by the model, but none of these are statistically significant.

Figure 3 also shows that the best-fitting XSTAR model is good at the O vi edge but could be better if the edge were deeper since the flux just above the edge is somewhat overpredicted. We note that the Fe ion columns predicted by the best-fitting XSTAR model are largest for ionization states Fe xiv to Fe xix (see Table 3). According to Behar, Sako, & Khan (2001), this should yield an Fe M-shell UTA in the energy region of interest. This has in fact been detected by XMM-Newton in Mrk 509 (Pounds et al. 2001), albeit at lower energy (centered at ~0.77 keV, rest frame; 0.744 keV, observed frame), corresponding to lower ionization states dominated by Fe xi–xii. Such UTAs have also been detected in some other Seyfert 1 galaxies (IRAS 13349+2438, Sako et al. 2001b; MCG –6-30-15, Lee et al. 2001; NGC 3783, Kaspi et al. 2002; NGC 5548, Kaatza et al. 2002). Fe L-shell absorption could also be present near the O vi (and the O viii edge) due to neutral Fe locked up in dust (see Fig. 3), and this is not modeled by XSTAR. Such a scenario was proposed by Lee et al. (2001) for MCG –6-30-15. However, we do not see evidence for these Fe L edges in Mrk 509, and this is consistent with the amount of reddening, which corresponds to a threshold optical depth of the neutral Fe L3 edge of ∼0.02, not detectable by the MEG. The complex of O vi 1s²–1snp resonance transitions with n > 5 may also complicate the region just above the O vi edge (see also Lee et al. 2001). We also point out that the data around ∼1.02–1.04 keV are not well fitted by the model (see Fig. 3). However, the break energy of the broken power law is at 1.04 keV (observed frame), and the break in the model spectrum is rather sharp, so a more physical model of the continuum may fit better.

The best XSTAR model absorber fit around the O vi edge and the Ne ix (r; λ13.447) absorption line (which is not far blueward of the O vii edge) is much better than the fit in the O vii edge region. In § 3 we mentioned how spectral fits using simple absorption-edge models (representing O vii and O viii) could be misleading. We see that more sophisticated modeling with better data now gives a smaller O vii edge since the data above the O vii edge are affected by other absorption features (Ne ix [r; λ13.447] in particular), which can be accounted for by the photoionization models. This has also been pointed out by Lee et al. (2001). However, the edge depth may still be overestimated due to the presence of Fe inner shell UTAs. From the XSTAR models we can extract the O vii and O viii ion column densities at the extremes of the 90% confidence intervals for N_H versus ξ. We find that the O vii column is 3.5 ±2.7 × 10^{17} cm^{-2} and the O viii column is 8.1 ±1.1 × 10^{17} cm^{-2}. Given an absorption cross section at a threshold of 2.75 × 10^{-19} and 1.09 × 10^{-19} cm² for O vii and O viii, respectively (Verner & Yakovlev 1995), we find that the model optical depths (at threshold) of the O edges are τ_{O vii} = 0.10^{+0.07}_{-0.05} and τ_{O viii} = 0.09^{+0.01}_{-0.02}, respectively. These values can be compared with those obtained from a Mrk 509 ASCA observation in 1994 in which simple “edge models” yielded τ_{O vii} = 0.11^{+0.04}_{-0.03} and τ_{O viii} = 0.04^{+0.03}_{-0.03} (Reynolds 1997; see...
also George et al. 1998). While the O vii optical depth is consistent, the O viii optical depth is only marginally consistent. However, variability of the warm absorber has been observed in several AGNs, and Mrk 509 may be no exception.

We investigated the robustness of the XSTAR model fits to the absorption features by examining the data versus model at the extremes of the \( N_H \) versus \( \xi \) confidence intervals (see Fig. 13). By picking pairs of values of \( N_H \) and \( \xi \) in the plane of the contours, we can freeze the column density and ionization parameter at the chosen values and find the new best fit for each pair of values (this is in fact how such contours are constructed). Then we can examine the data and model spectra in detail for each of these new fits to see where the model and data deviate significantly from each other. We found that the models were still able to account for the strengths of all of the strong absorption-line features (listed in Table 1) for pairs of \( N_H \) and \( \xi \) lying inside the 68\% confidence contour. On the other hand, for pairs of \( N_H \) and \( \xi \) lying near the 99\% contour, we found that the Ne x Ly\( \alpha \) (\( \lambda 12.134 \)) absorption line was particularly sensitive, and the equivalent width would be overpredicted or underpredicted by as much as a factor of 2. Therefore, we conclude that the confidence contours in Figure 13 are conservative and that the true parameter space for the allowed range of \( N_H \) and \( \xi \) is even more restricted than the 99\% confidence contours in Figure 13 indicate.

5.5. Emission-Line Spectra

As well as absorption, the XSTAR code also calculates emission spectra assuming a shell of gas subtending 4\( \pi \) sr at the central ionizing source. The fact that we do not detect any strong, identifiable emission features does not place constraints directly on the covering factor since we do not know the gas density or its distance from the ionizing source. Requiring that the shell of gas be much thinner than its distance to the source (i.e., \( \Delta r/r \ll 1 \)) and using the best-fitting values of column density and ionization parameter constrain the upper limit on the absorber distance only on the order of kiloparsecs (e.g., see Turner et al. 1993).

It has been argued in the literature, based on XMM-Newton RGS grating data, that the soft X-ray spectra of MCG –6-30-15 and Mrk 766 can be better explained by relativistically broadened emission lines due to C vii Ly\( \alpha \) (\( \lambda 33.736 \)), N vii Ly\( \alpha \) (\( \lambda 24.781 \)), and O viii Ly\( \alpha \) (\( \lambda 18.969 \)) rather than by a pure photoionized absorber (e.g., Branduardi-Raymont et al. 2001; however, see Lee et al. 2001 for counterarguments). Because of the different MEG bandpass, we can test only for relativistically broadened O viii Ly\( \alpha \) (\( \lambda 18.969 \)) emission in our Mrk 509 data. First, we note that we cannot obtain even a reasonable spectral fit with only a relativistic disk line and no warm absorber. When we added an emission-line model from a relativistic disk around a Schwarzschild black hole (e.g., Fabian et al. 1989) to the best-fitting photoionized absorber model, we obtained a reduction in the C-statistic corresponding to only 90\% confidence for the addition of two free parameters (the disk inclination and line intensity). The inner and outer radii of the disk were fixed at 6 and 1000 gravitational radii, respectively, and the radial line emissivity per unit area was a power law with index –2.5. The line energy was fixed at 0.65362 keV in the Mrk 509 rest frame. The best-fitting inclination angle and equivalent width was 41\(^\circ\) and 17 ± 9 eV, respectively. Pounds et al. (2001) assumed an inclination angle of 30\(^\circ\) when fitting ionized disk reflection models, and in Paper II we also argue for a small inclination angle. If we fix the disk inclination at 30\(^\circ\) in the Chandra fit, we find a much smaller equivalent width of 8\(^+5\) eV. When the O viii Ly\( \alpha \) (\( \lambda 18.969 \)) emission line is included in the model, the best-fitting XSTAR model of the absorber does not change much: \( \log \xi \) decreases from 1.76 to 1.65 and \( N_H \) decreases by ~13\% to \( 1.80 \times 10^{23} \) cm\(^{-2} \). We caution that in our case the broad line may simply be modeling residuals that are remaining calibration uncertainties and/or curvature in the spectrum and conclude that the evidence for relativistically broadened O viii Ly\( \alpha \) (\( \lambda 18.969 \)) emission in our data is not compelling but not ruled out either.

5.6. Effects of Changes in the SED

To investigate the effect of uncertainty in the energy range \( \sim 10–500 \) eV in our fiducial SED, we generated XSTAR models using alternative SEDs in the manner described for the fiducial SED (see § 5.1). Two alternative SEDs were used, in which the flux at 55 eV was either 50\% lower or 50\% higher relative to the fiducial SED. These SEDs are illustrated by dashed lines in Figure 10. Proceeding with model-fitting just as described for the fiducial SED, we found that the best-fitting column density (\( N_H \)), ionization parameter (\( \xi \)), soft power law photon index, and broken power law break energy were consistent for all three SEDs, within the statistical errors. Moreover, the models with the alternative SEDs were able to provide fits to all the major discrete absorption features and edges that were just as good, or no worse, than the fiducial SED models. We also found that the predicted ionic columns of O vii and O viii for the best-fitting models using the alternative SEDs did not differ by more than 10\% from the values obtained with the baseline SED model. Thus, our results and conclusions are not sensitive to any reasonable uncertainties in the unobserved EUV part of the SED.

6. COMPARISON WITH AN XMM-NEWTON OBSERVATION IN 2000 OCTOBER

Mrk 509 was observed by XMM-Newton on 2000 October 25 (Pounds et al. 2001), ~180 days before our Chandra HETGS observation. In this section we compare our Chandra results to the XMM-Newton results for the soft X-ray spectrum of Mrk 509. The Fe K region and higher energy spectrum has already been discussed in detail and compared to the XMM-Newton results in Yaqoob et al. (2002). Several factors need to be borne in mind when making the comparison of the soft X-ray spectra. First, the effective areas of the XMM-Newton gratings (RGS) exceed that of the Chandra MEG below ~1.15 keV. Second, the spectral resolution of the RGS at 0.5 keV is at best ~850 km s\(^{-1} \) (compared to ~280 km s\(^{-1} \) for the MEG). The spectral resolution in both cases is worse at higher energies. Third, the exposure times for the XMM-Newton CCDs were ~25–27 ks and ~30 ks for the RGS. This is to be compared to ~58 ks for the Chandra exposure time. Fourth, the 0.5–10 keV observed flux during the XMM-Newton observation was \( 2.6 \times 10^{-11} \) ergs cm\(^{-2} \) s\(^{-1} \), a factor of 2.8 less than the corresponding MEG 0.5–10 keV flux of \( 7.3 \times 10^{-11} \) ergs cm\(^{-2} \) s\(^{-1} \).

XMM-Newton and Chandra observed a similar underlying continuum. The EPIC XMM-Newton CCD data yielded
a 2–10 keV power-law index of 1.66 ± 0.02, in good agreement with our Chandra/RXTE measurements of 1.674±0.010 (Yaqoob et al. 2002). A strong soft excess relative to this power law was observed by both XMM-Newton and Chandra and with a similar magnitude relative to the hard power law. Pounds et al. (2001) report detecting only two significant absorption features, namely, a blend of Ne ix (r) and Fe xix at 13.52 Å and a broad absorption trough, likely to be associated with an Fe M-shell UTA, centered around 16.1 Å. According to the calculations of Behar et al. (2001), this corresponds to ionization states dominated by Fe xi–xii. The Ne ix (r; λ13.447) feature was detected by the MEG, and our data are not inconsistent with the Fe M-shell UTA. We established the latter by adding a Gaussian absorption trough to our best-fitting XSTAR model, in order to model the UTA (using the parameters measured by Pounds et al. 2001), and found that the agreement between data and model improved and that the data did not deviate by more than one standard deviation from the model in the 0.70–0.78 keV region (observed). At the Ne ix / Fe xix feature the underlying continuum was a factor of ~2 higher during the Chandra observation than in the XMM-Newton observation. The equivalent widths of the Ne ix /Fe xix absorption features (1.0 ±0.5 eV for Chandra, 2.2 ± 1.0 eV for XMM-Newton) are compatible with the absorption responding to the change in continuum level, as would be expected. Since Pounds et al. (2001) do not give any further measurements or limits (in particular, on the O viii and O vii edges) or results of photoionization modeling, it is difficult to make a more detailed comparison of the warm absorber during the two observations.

Pounds et al. (2001) also detected O viii He-like triplet emission in the RGS data, with the intercombination line being the strongest (equivalent width 1.5 ± 0.7 eV). Smaller equivalent widths of the O vi–He-like triplet emission lines in the Chandra MEG data would be expected if the intensity of the emission lines remained constant while the underlying continuum increased (by more than a factor of 2 in this case). None of the O vii triplet lines are detected significantly, most likely due to insufficient SNR. For example, at the energy of the O vii 1s2–1s2p resonance line, the combined effective area of the two RGS instruments on XMM-Newton is a factor of ~60 higher than the MEG. Combined with the shorter exposure and lower source flux for the XMM-Newton observation, the SNR of the RGS data at the O vii 1s2–1s2p resonance line is a factor of ~3 higher than in the MEG data. Nevertheless, we do obtain a non-zero intensity from Gaussian modeling of the MEG data. Direct measurement of the intercombination line in the MEG data gives an equivalent width of 1.00±0.44 eV. Unfortunately, the SNR is insufficient to determine whether the emission-line intensity did or did not respond to the change in the continuum, so we cannot constraint the distance of the emitter.

7. RELATION BETWEEN THE X-RAY AND ULTRAVIOLET WARM ABSORBERS

Our Chandra HETGS observation was simultaneous with an HST/STIS observation. Full details of the results from the UV data are discussed in Paper II. Here we simply summarize very briefly the findings of Paper II and discuss whether the UV absorption predicted by our simple model of the X-ray absorber is consistent with the UV data.

The HST/STIS spectrum of Mrk 509 shows multiple kinematic components to the UV absorption features, a characteristic that is found to be common in Seyfert 1 galaxies (e.g., Crenshaw & Kraemer 1999). Specifically, eight distinct kinematic components are identified for C iv, N v, and Si iv. The seven principal kinematic components (numbered 1 through 7 in Paper II) lie at ~422, ~328, ~259, ~62, ~22, +34, and +124 km s⁻¹, respectively, relative to systemic. Figure 9 shows the UV absorber velocities superimposed on some of the strongest absorption features in the Chandra HETGS data, along with the best-fitting XSTAR photoionization model profiles. Shown are the velocity profiles of Ne x Lyα (λ121.34), Ne ix (r) 1s²–1s2p (λ13.447), Mg xi (r) 1s²–1s2p (λ11.547), and O viiι Lyα (λ18.969). The UV kinematic components are clipped into two groups and together clearly span the widths of the X-ray profiles. It is possible that these X-ray velocity profiles actually consist of several kinematic components that cannot be resolved by Chandra. We convolved the UV kinematic components through the MEG response function and found the resulting profiles to be compatible with the observed X-ray profiles. The observed X-ray profiles of Ne ix (r) 1s²–1s2p (λ13.447) and Mg xi (r) 1s²–1s2p (λ9.169) appear to be somewhat different from those of Ne x Lyα (λ121.34) and O viii Lyα (λ18.969), the former pair being somewhat asymmetric. As pointed out in §§ 4 and 5, this could be due to blending with unresolved line emission. Alternatively, the profiles could be intrinsically different. However, we again caution that the velocity resolution of the X-ray profiles shown in Figure 8 is between ~350 and 730 km s⁻¹ FWHM, so the differences in the X-ray profiles must be regarded as tentative.

Although the X-ray and UV absorbers may share the same velocity space, in Paper II we show that the ionization state and column densities of the UV absorbers are too low to produce the observed X-ray absorption. Photoionization models for each of the UV kinematic components yielded column densities, N_H, in the range 1.77×10^{18} to 4.00×10^{19} cm⁻² and log Γ in the range 0.01 to 1.33 (or log U in the range ~1.48 to ~0.16). Conversely, the column density and ionization parameter of the X-ray absorber is high. The best-fitting parameters from photoionization modeling of the X-ray data are log Γ = 1.76 (log U = 0.27) and N_H = 2.06×10^{21} cm⁻². Some UV absorption is predicted by the best-fitting XSTAR model to the Chandra data, but the relevant ionic column densities are small enough that the predictions of the X-ray model are not in conflict with the UV data. Table 3 gives some column densities of some key ions from our best-fitting photoionization model to the X-ray data, compared with some measured column densities from the UV data, as well as some corresponding predicted column densities from the UV photoionization modeling. Indeed, it can seen that in the X-ray absorber, the predicted column densities of C ii, C iii, C iv, N v, and O vi could easily be hidden in the UV absorbers. Full details, including a plausible physical and geometrical picture of the X-ray and UV absorbers, can be found in Paper II.

8. CONCLUSIONS

We observed Mrk 509 for ~59 ks with the Chandra HETGS on 2001 April 13–14, simultaneously with RXTE and HST/STIS. The complex Fe K line and Compton-
reflection continuum are discussed in Yaqoob et al. (2002). Details of the UV data and results from the HST/STIS observation are given in Paper II. Here we summarize the main results from the Chandra HETGS soft X-ray spectrum, in view of relevant constraints from the RXTE and HST/STIS observations.

1. Combined Chandra MEG and HEG and RXTE data show that the hard X-ray spectrum of Mrk 509 is well described by a simple power law, with little Compton-reflection continuum required, and a photon index of $\Gamma = 1.67$ above 2 keV. At lower energies, below $\sim 1$ keV, the spectrum steepens, the soft excess attaining a magnitude of about 60% higher than the extrapolated hard power law. When the intrinsic X-ray continuum is modeled with a broken power law, self-consistently modeling the X-ray absorption with a photoionization model (see below) yields a break energy $E_B = 0.95^{+0.15}_{-0.09}$ keV and a soft power law index of $\Gamma = 2.36^{+0.21}_{-0.20}$. During the observing campaign the broadband source flux was $5.1 \times 10^{-11}$ ergs cm$^{-2}$ s$^{-1}$, typical of historical values (the corresponding 2--10 keV luminosity was $1.3 \times 10^{44}$ ergs s$^{-1}$).

2. Below $\sim 2$ keV, the observed spectrum shows considerable deviations from a smooth continuum, due mainly to bound-free absorption opacity, and complexes of discrete absorption features. Particularly noteworthy are the O vii and O viii edges at 0.732$^{+0.004}_{-0.019}$ and 0.871$^{+0.014}_{-0.020}$ keV, respectively. Within the errors, both values are consistent (O vii marginally so) with their respective rest energies, and from the best-fitting photoionization models the optical depths at threshold are $0.10^{+0.05}_{-0.04}$ for O vii and $0.09^{+0.07}_{-0.01}$ for O viii. Compared with a previous ASCA observation (Reynolds 1997; George et al. 1998), the O vii edge is consistent, while the O viii edge is somewhat larger in the MEG data. However, we note that the edge depths may be variable in some AGNs (e.g., Otani et al. 1996; Guainazzi et al. 1996). Estimates of the O vii edge depth are also complicated by nearby absorption features due, for example, to Ne and Fe. The spectral region between the O vii and O viii edges is very complex and the most difficult to model with a simple photoionized absorber. This part of the spectrum is also where one would expect Fe L edges (e.g., due to dust) and Fe M-shell UTAs, neither of which are detected. The data are, however, consistent with a UTA with model parameters measured during an XMM-Newton observation (Pounds et al. 2001).

3. On the next level of detail, we detect absorption lines from H-like ions of N, O, and Ne, He-like ions of O, Ne, and Mg, as well as absorption features due to highly ionized Fe. The ionization state of the absorber is high, but not so high that absorption due to H-like Mg or Si is detected. Only the Ne x Ly$\alpha$ (A12.134) and Ne ix 1s$^2$-1s2p lines appear to be marginally resolved, and the rest are unresolved (FWHM < 300 km s$^{-1}$ for N, going up to FWHM < 1330 km s$^{-1}$ for Mg). The absorption lines are consistent with an outflow of $-200$ km s$^{-1}$ relative to systemic. However, the detailed velocity profiles of the absorption features are not all the same for all ionic species. The complexity and differences in profiles could be due to the contribution from different, unresolved kinematic components and/or blending and contamination from absorption/emission due to other atomic transitions.

4. We have modeled the Chandra HETGS spectra using the photoionization code XSTAR, version 2.1.d, with an SED constructed using our UV and X-ray data. The best-fitting ionization parameter and neutral equivalent hydrogen column density of the absorbing gas are $\log \xi = 1.76^{+0.13}_{-0.11}$ ergs cm s$^{-1}$ (or $\log U = 0.27$) and $N_H = 2.06^{+0.39}_{-0.35} \times 10^{21}$ cm$^{-2}$, respectively. This best-fitting model gives an excellent fit to the overall observed spectrum. It also is able to model all the principal local absorption features to a degree ranging from fair to excellent, except for the region around 0.78--0.80 keV. The poor fit here may be, in part, due to uncertainties in the instrument response function. A curve-of-growth analysis indicates that a velocity width of $b = 100$ km s$^{-1}$ gives a good match to measured absorption-line equivalent widths. Our results are insensitive to reasonable uncertainties in the unobserved EUV part of the SED.

5. We do not detect any clearly identifiable emission lines (apart from the Fe K line), in contrast with an earlier XMM-Newton observation in which Pounds et al. (2001) detected He-like O viii triplet emission, which constrained the electron density to be greater than $10^{11}$ cm$^{-3}$. However, this lower limit is subject to uncertainties in the line-ratio measurements. Although the broadband X-ray flux during that observation was nearly a factor of 3 lower than it was during our campaign, the SNR of our data is worse and insufficient to constrain the distance of the emitter from the ionizing source. Since we cannot assume that the emitter and absorber have the same ionization state and/or column density, time-resolved spectroscopy with better SNR is required to address the question of the location of the absorber and emitter. Deducing the mass outflow of the X-ray absorber must also await better data because the density and global covering factor are unknown.

6. Simultaneous HST/STIS observations of Mrk 509 indicate that there are eight kinetic components comprising the UV absorbers, with velocities ranging from $-422$ to $+124$ km s$^{-1}$. The X-ray absorber is compatible with sharing the same velocity space as the UV absorbers. It is possible that the velocity profiles of the X-ray absorbers are also made up of several kinematic components, possibly the same as the UV ones, but unresolved because of the factor of greater than 30 worse velocity resolution of the X-ray data compared to the UV data. The X-ray profiles do, however, hint at complex structure, possibly two kinematic components or groups of components. The UV components certainly appear to cluster into two groups. There are also differences in the X-ray velocity profiles between some of the ion species. This may be due to genuine differences in gasdynamics but may also be due to unresolved and unmodeled line emission. On the other hand, other Seyfert 1 galaxies also show two kinematic components (or groups of components) in their absorption-line profiles, but with different offsets relative to systemic (NGC 5548, Kaastra et al. 2002; NGC 4051, Collinge et al. 2001; NGC 3783, Kaspi et al. 2002).

7. Although the X-ray and UV absorbers may share the same velocity space, Paper II shows that the ionization state and column densities of the UV absorbers are too low to produce the observed X-ray absorption. Conversely, the ionization and column density of the X-ray absorber is high; some UV absorption is predicted by our best-fitting photo-ionization model to the Chandra data, but the relevant ion column densities can be hidden in the UV absorbers.
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