## SOFT X-RAY OPACITY IN HOT AND PHOTOIONIZED GASES

JULIAN H. KROLIK<sup>1</sup>
Harvard-Smithsonian Center for Astrophysics

AND

TIMOTHY R. KALLMAN<sup>2</sup>
NASA/Goddard Space Flight Center
Received 1984 February 3; accepted 1984 May 24

### **ABSTRACT**

New calculations are presented of the soft X-ray opacity of gas having cosmic elemental abundances, but in a variety of ionization states. We consider coronal ionization equilibrium over the range of temperatures  $10^4$  to  $3\times 10^8$  K and photoionization equilibrium with power-law and thermal bremsstrahlung spectra over a wide range of ionization parameters. The results are displayed in illustrative figures. For temperatures and ionization parameters commonly found in astrophysical plasmas, the opacity (particularly to photons of  $\leq 1$  keV) can be diminished by substantial factors relative to the state in which all atoms are neutral. As the dominant ionization stages change, the positions and contrasts of prominent K-edges also change.

Subject headings: atomic processes — opacities — plasmas — X-rays: spectra

#### I. INTRODUCTION

Shortly before the launch of the first X-ray astronomy satellite, Brown and Gould (1970) published the first thorough calculation of the opacity of cosmic plasmas to soft X-radiation. They assume that all the elements were present in their cosmic abundances, and that all atoms were neutral. Subsequently, Fireman (1974) calculated the modifications to their results produced by the self-shielding of certain elements (principally oxygen) inside interstellar dust grains. Ride and Walker (1977) and Morrison and McCammon (1983) have performed calculations similar to that of Brown and Gould, but using more recent atomic data.

These calculations have proven extremely useful to the interpretation of soft X-ray spectral data, but they are incomplete, for they fail to take into account the modification of the opacity due to ionization of the absorbing atoms. Ionization alters the soft X-ray opacity in two ways. First, in stages of partial ionization, the energies of the K-shell edges increase and the cross sections to photoionization decrease with respect to the neutral atoms as electron shielding becomes less important (Daltabuit and Cox 1972). Second, when atoms are shorn of all their electrons, they are no longer capable of absorbing X-rays at all, while their scattering cross section is reduced to the product of their atomic number and the Thomson cross section. Thus, in general, increasing ionization decreases the opacity.

However, the decrease in opacity does not proceed uniformly at all photon energies. Because the opacity to the softest X-ray photons is dominated by atoms and ions with the lowest ionization potentials, the opacity to soft X-ray photons diminishes more at lower temperatures and ionization parameters than that of harder photons. Consequently, the spectrum of X-rays which have passed through an absorbing medium may show signs of moderate absorption over a broad range of photon energies, rather than very strong absorption at low

<sup>2</sup> Also Department of Physics and Astronomy, University of Maryland.

energies and virtually no absorption at high energies, as is commonly expected.

In this paper we present a careful, quantitative treatment of how the absorption opacity changes as a function of temperature and degree of ionization. We give only the absorption opacity for two reasons: scattering may or may not reduce the received flux, depending on whether the scattering medium lies within the telescope beam; and except for a small number of resonance lines, the scattering opacity is essentially trivial to calculate for plasmas such as these, for it is just the electron density times the Thomson cross section.

Our results will be of interest for the interpretation of soft X-ray spectra in a great variety of objects, for the typical state of cosmic gas is to be at least partially ionized. The majority of the volume in our own Galaxy is taken up by a phase of the interstellar medium whose temperature is  $\sim 3 \times 10^5$  K (Cox and Smith 1974; McKee and Ostriker 1977); compact binary X-ray sources often exhibit hot coronae through which the central source's radiation must pass (White and Holt 1982); X-ray emitting hot stars' ultraviolet spectra reveal the presence of highly ionized species such as O<sup>+5</sup> and C<sup>+3</sup>, while their X-ray spectra show evidence for absorption (Cassinelli et al. 1981); active galaxies contain both clouds photoionized to temperatures  $\sim 10^4$  K which sometimes lie along the line of sight to the X-ray continuum source, and other gas which almost certainly lies in the line of sight and which is probably hotter than 106 or 107 K (Krolik, McKee, and Tarter 1981; McKee and Shields 1981; Holt et al. 1980; Petre et al. 1984). In all these instances, the ionization state of the principal absorbing elements is far enough from neutral to alter the opacity by factors of at least several, and sometimes by orders of magnitude.

The photoionization code which we have used to obtain these results is the one described in Kallman and McCray (1982). This calculation is based on the assumption of a local balance between the various heating and cooling, and ionization and recombination, processes affecting the gas. These processes include: photoionization and photoionization heating, collisional ionization and excitation, radiative and die-

<sup>&</sup>lt;sup>1</sup> Supported in part by NSF grant 80-07351 and by subcontract 9744809 with the University of California Lawrence Livermore Laboratory.

lectronic recombination, charge transfer recombination by H and He along with the associated cooling, heating and cooling by Compton scattering, and bremsstrahlung cooling. Photoionization cross sections were taken from Reilman and Manson (1978, 1979); Barfield, Koontz, and Huebner (1972); and Huebner, Argo, and Ohlsen (1978). Our recombination rates are from Aldrovandi and Pequinot (1973). We used ECIP (exchange classical impact parameter: Summers 1974a, b; Burgess and Summer 1976) rates for collisional ionization (Sarazin 1978). The merits of these rates and their derivation are discussed in detail by Hamilton, Sarazin, and Chevalier (1983). Butler, Heil, and Dalgarno (1980) and Dalgarno, Heil, and Butler (1981) were our sources for charge transfer rates. Kato (1976), Stern, Wang, and Bowyer (1978), Gau and Henry (1977), and various other references summarized in Kallman and McCray (1982) were used for collisional excitation rates. Our code assumes the abundances tabulated by Withbroe (1971): relative to the number of H atoms, there are 0.1 He atoms,  $3.8 \times 10^{-4}$  C atoms,  $8.7 \times 10^{-5}$  N atoms,  $4.4 \times 10^{-4}$  O atoms,  $2.6 \times 10^{-5}$  Ne atoms,  $3.0 \times 10^{-5}$  Mg atoms,  $3.2 \times 10^{-5}$  Si atoms,  $1.4 \times 10^{-5}$  S atoms, and  $3.2 \times 10^{-5}$  Fe atoms.

Whenever the ionization state of the plasma is affected by external radiation, we assume that the plasma is optically thin to the ionizing radiation. There is little that can be said about the validity of this approximation when the ionizing radiation is independent of the X-ray continuum whose absorption is at issue, except that it is, of course, the simplest case. When the ionizing radiation is associated with the observed X-ray continuum, the maximum column density at which the approximation is valid may be determined post hoc from our calculations.

### II. CORONAL IONIZATION EQUILIBRIUM

Figure 1 shows the opacity to photons between 100 eV and 10 keV presented by a plasma with cosmic abundances in coronal ionization equilibrium, for temperatures 10<sup>4</sup> K, 10<sup>5</sup> K, 106 K, and 107 K. The opacity to photons throughout this band is negligible at temperatures 108 K and higher.

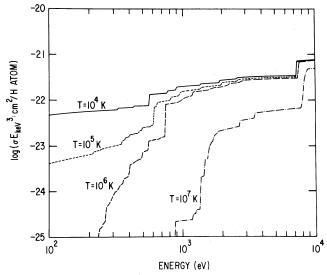


Fig. 1.—The opacity per hydrogen atom times  $(\epsilon/keV)^3$  as a function of photon energy for various temperatures, assuming coronal ionization equi-

At 10<sup>4</sup> K, the opacity is essentially at the neutral atom limit. However, at temperatures only slightly higher ( $\sim 2 \times 10^4$  K), hydrogen becomes mostly ionized, and the opacity to photons of a few hundred eV begins to drop (helium, which is still predominantly neutral at this temperature, is the greatest single contribution to the opacity, or the diminution would be greater). By  $3 \times 10^4$  K, the opacity in this range is diminished by roughly a factor of 2, as the abundance of He<sup>+</sup> and He<sup>+</sup> increases. At a temperature of 10<sup>5</sup> K, so little He and He<sup>+</sup> remain that the very soft X-ray opacity becomes dominated by carbon; but by then, the carbon is 2-4 times ionized, and its K-edge has moved up to 344-399 eV. Below 344 eV such plasmas are virtually transparent, while above that threshold, the opacity is nearly the same as the neutral limit value.

The principal feature of the 0.5-1 keV band, the oxygen K-edge, slowly increases in energy and in contrast as the temperature rises. In neutral oxygen, the edge is at 533 eV, but charge exchange ties the abundance of O+ to that of H+, so that at  $2 \times 10^4$  K oxygen is mostly singly ionized and the edge moves to 580 eV. When only one electron remains bound to the oxygen ions (a condition which is reached around 10<sup>6</sup> K), the edge rises to 870 eV. Below this edge, the opacity falls substantially as the temperature rises above 10<sup>4</sup> K because hydrogen and helium, the dominant contributors to the opacity, become progressively more and more fully stripped. But, until oxygen itself becomes mostly fully stripped (at a temperature of  $\sim 3 \times 10^6$  K), the opacity to photons above the oxygen K-edge drops only slowly. Consequently, the contrast across the edge (i.e., the ratio of opacity immediately above the edge to that immediately below) increases steadily from 10<sup>4</sup> K to  $3 \times 10^6$  K. An analogous mechanism strengthens the contrast of the silicon ( $\approx$ 2 keV) and sulfur ( $\approx$ 2.5 keV) edges in the temperature range around  $10^6-10^7$  K, and the iron edge (7-8.5 keV) from  $10^5$  K all the way up to  $3 \times 10^8$  K.

When the temperature is 10<sup>7</sup> K or higher, gas of cosmic abundances is almost transparent to photons below 2 keV. In the range of temperatures from 10<sup>7</sup> to 10<sup>8</sup> K, photons in the range 2-6 keV face an opacity roughly an order of magnitude less than the neutral gas value, as only higher-Z elements (chiefly Mg and Si) retain any electrons. Above the Fe K-edge (roughly 7-9 keV, depending on which ionization stage), the opacity does not diminish until the temperature rises above  $10^{8} \, \mathrm{K}$ 

Figure 2 presents some of the same data in a different format. Here we show the opacity decreases with temperature at specific photon energies. Typically, one element provides most of the opacity at any given energy, so the opacity decreases slowly with temperature below some critical value at which that element becomes fully stripped, and drastically above that value.

# III. PHOTOIONIZATION EQUILIBRIUM

To illustrate the opacity properties of plasmas in photoionization equilibrium, we present data for spectra of two different shapes. While the results for the two examples share basic similarities, the contrast in spectral shape does introduce significant differences in detail. These differences are in general great enough that, in order to evaluate the opacity in a plasma photoionized by a given spectrum, it is necessary to make a calculation specific to that spectrum.

The first example is a power-law spectrum in which the energy flux per photon energy is proportional to  $\epsilon^{-1}$ , the reciprocal of the photon energy, between 1 eV and 400 keV.

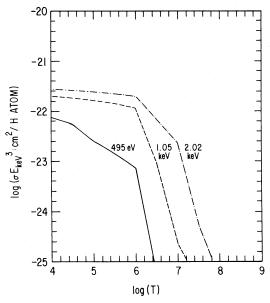


Fig. 2.—The same vertical scale as Fig. 1, but plotted as a function of temperature for several photon energies, also in the case of coronal ionization equilibrium.

This shape is a crude approximation to the typical spectra of quasars and Seyfert galaxies (Rothschild *et al.* 1983). Figure 3 shows the equilibrium temperature T as a function of the ionization parameter  $\Xi = L/(4\pi c r^2 n_{\rm H} \, kT)$ . As is characteristic of such spectra, the temperature as a function of  $\Xi$  is almost constant at  $\sim 10^4$  K below a critical value (here  $\sim 10$ ) and climbs very steeply to the Comptonization temperature (here almost  $10^8$  K) for larger values of  $\Xi$  (Krolik, McKee, and Tarter 1979). In between, where the curve doubles back, there are equilibria which are unlikely to be found in nature because they are unstable to isobaric perturbations.

The opacity curves for four sample equilibria are shown in Figure 4. Their positions on the  $T-\Xi$  equilibrium curve of

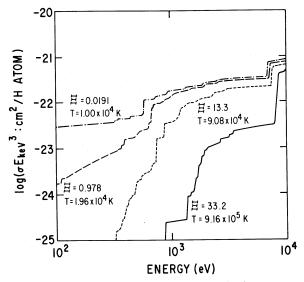


Fig. 4.—The opacity per hydrogen atom times  $(\epsilon/\text{keV})^3$  as a function of photon energy for various photoionization equilibria, assuming an incident power-law spectrum of index-1.

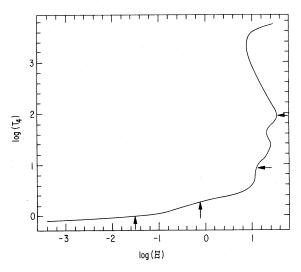


Fig. 3.—The photoionization equilibrium temperature as a function of ionization parameter  $\Xi$  for a continuum spectrum of power-law index-1. The arrows mark the points for which the opacity is displayed in Fig. 4.

Figure 3 are marked with arrows. All are stable to isobaric perturbations.

When  $\Xi$  is less than  $\approx 0.03$  (corresponding to  $T \approx 8 \times 10^3$  K), the opacity is well described by the neutral atom limit. Above that value of  $\Xi$ , even though the temperature remains near  $10^4$  K, the opacity decreases, with the largest effects at the lowest photon energies. As we explained in the case of coronal ionization equilibrium, the opacity below 500 eV is ordinarily dominated by H and He, and falls as their neutral fractions fall.

The opacity between 500 and 800 eV also falls as  $\Xi$  increases above 0.03, as the dominant ionization state of oxygen becomes one with fewer and fewer electrons and the position of the oxygen edge shifts to higher energies. Even at temperatures as low as  $2 \times 10^4$  K, the opacity at 600 eV, for example, is diminished by an order of magnitude with respect to the neutral atom limit. For the same reason as in the coronal equilibrium case, the contrast of the oxygen edge (and to a lesser degree, those of Si and S) is greatly enhanced in the temperature range  $10^4-10^5$  K. The ratio of opacity immediately above the edge to that immediately below rises from  $\approx 2$  at the lower end of this range to  $\approx 6$  at the upper.

On the portion of the T- $\Xi$  curve which is almost vertical ( $\Xi \approx 10$ ), the opacity drops dramatically as T increases: by  $10^5$  K, gas is almost transparent to all photons below 1 keV, and is 2-5 times less opaque than neutral gas from 1 keV to the Fe K-edge at approximately 7 keV. At  $10^6$  K, the opacity is reduced by nearly two orders of magnitude for photons below the Fe K-edge, which has meanwhile risen to 8.5 keV. By the time the next stable equilibrium appears (at a little over  $10^7$  K), even Fe absorption has disappeared.

For our second photoionization equilibrium example we have chosen a 2 keV thermal bremsstrahlung spectrum. Spectra of this sort are commonly emitted from pre-main-sequence stars, for example (Feigelson 1984), while somewhat harder exponential spectra are characteristic of compact binary X-ray sources and the gas in clusters of galaxies. Figure 5 shows the equilibrium temperature as a function of  $\Xi$ . As in

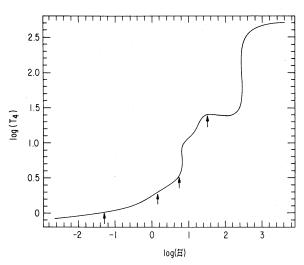


Fig. 5.—The photoionization equilibrium temperature as a function of ionization parameter  $\Xi$  for a 2 keV optically thin bremsstrahlung spectrum. The arrows mark the points for which the opacity is displayed in Figure 6.

the  $\epsilon^{-1}$  case, T rises sharply for  $\Xi \ge 10$ . However, unlike the  $\epsilon^{-1}$  case, there is a stable equilibrium over a fairly broad range of  $\Xi$  with  $T \approx 3 \times 10^5$  K, and there are no regions (except for two very narrow bands at  $\Xi \approx 6$  and 250) in which unstable equilibrium exist. In a further contrast with the  $\epsilon^{-1}$  case, the highest temperature equilibrium lies at only  $\sim 5 \times 10^6$  K.

Again, the opacity at the equilibrium points picked out by arrows is shown in the accompanying figure, Figure 6. The behavior of the opacity as a function of T and  $\Xi$  is qualitatively similar to the  $\epsilon^{-1}$  case, but differs significantly in detail. To achieve a similar level of ionization, the bremsstrahlung spectrum requires a higher ionization parameter, but this higher ionization parameter produces a lower temperature. The contrast is due to the larger portion of the bremsstrahlung spectrum's energy that is tied up in energetic photons of small cross section. These contribute to  $\Xi$  but are relatively ineffective as agents of photoionization.

Just as in the power-law case, the opacity below 500 eV drops rapidly through the range of  $\Xi$  in which the temperature is  $\sim 10^4$  K. By the time a temperature of  $3\times 10^4$  K is achieved, the plasma is almost transparent to photons below the oxygen edge, even though the opacity above the edge has only been altered very slightly. Again, the position of the oxygen edge moves upward through this temperature range, and its contrast increases.

The greatest contrast between the power-law and bremsstrahlung spectra comes at somewhat larger  $\Xi$ . In order to decrease the 1–6 keV opacity by two orders of magnitude in the former case, it is necessary to reach temperatures approaching  $10^6$  K. In the latter case, such a reduction occurs at smaller temperature, around  $3 \times 10^5$  K. The reason is again that the same ionization parameter produces a lower temperature when the spectrum is X-ray bremsstrahlung than when it is  $\epsilon^{-1}$  power-law, but its effectiveness as an ionizing agent can be almost as great.

The Fe edge disappears in the case of this bremsstrahlung

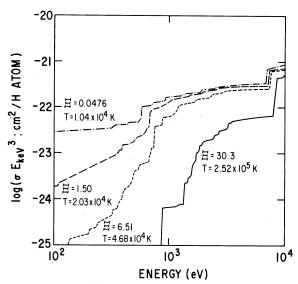


Fig. 6.—The opacity per hydrogen atom times  $(\epsilon/\text{keV})^3$  as a function of photon energy for various photoionization equilibria, assuming an incident 2 keV opacity thin bremsstrahlung spectrum.

spectrum at relatively low temperature (between the stable equilibria at  $3 \times 10^5$  K and  $3 \times 10^6$  K) because the highest temperature possible, the Comptonization temperature, is also relatively low, only  $\sim 5 \times 10^6$  K.

# IV. CONCLUSIONS

We have explicitly shown how the soft X-ray opacity of gas with cosmic abundances declines as it is heated and photoionized. This reduction in opacity is significant in the interpretation of soft X-ray spectra because the gas that the X-rays pass through is very often either sufficiently hot or sufficiently ionized that its opacity, particularly below 1 keV, is significantly less than that predicted in the neutral atom limit.

The principal effects of progressively greater ionization are as follows:

- 1. At relatively low temperatures, the ionization of hydrogen and helium makes plasmas nearly transparent to photons below the oxygen edge, while the opacity above that edge is almost unchanged.
- 2. In the range of temperatures in which the hydrogen and helium disappear, the oxygen edge moves from 533 eV to 870 eV, and its contrast (ratio of opacity immediately above to immediately below) increases.
- 3. At somewhat higher temperatures, oxygen becomes fully stripped, decreasing the total opacity above 1 keV substantially, and intensifying the contrast of the Si and S K-edges.
- 4. Ultimately, only Fe is left as a significant agent of opacity. It, too, ultimately disappears at a temperature determined by the dominant ionization processes, but which can be as low as  $\sim 10^6$  K.

We recognize that for any specific case, the figures we present here are unlikely to be adequate for proper data analysis. We therefore offer our computing assistance to anyone wishing to analyze soft X-ray spectra along the lines we have discussed here.

### KROLIK AND KALLMAN

#### REFERENCES

Aldrovandi, S., and Pequinot, D. 1973, Astr. Ap., 25, 137.

Barfield, W. C., Koontz, G. D., and Huebner, W. F. 1972, J. Quant. Spectrosc. Rad. Transf., 12, 1409.

Brown, R. L., and Gould, R. J. 1970, Phys. Rev. D, 1, 2252.

Burgess, A., and Summers, H. P. 1976, M.N.R.A.S., 174, 345.

Butler, S., Heil, T. G., and Dalgarno, A. 1980, Ap. J., 241, 442.

Cassinelli, J. P., Waldron, W. L., Sanders, W. T., Harnden, F. R., Jr., Rosner, R., and Vaiana, G. S. 1981, Ap. J., 250, 677.

Cox, D. P., and Smith, B. W. 1974, Ap. J. (Letters), 189, L105.

Dalgarno, A., Heil, T. G., and Butler, S. 1981, Ap. J., 245, 793.

Daltabuit, E., and Cox, D. P. 1972, Ap. J., 177, 855.

Feigelson, E. 1984, in Cool Stars, Stellar Systems, and the Sun, ed. S. L. Baliunas and L. Hartmann (Berlin: Springer), p. 27.

Fireman, E. L. 1974, Ap. J., 187, 57.

Gau, J. N., and Henry, R. J. W. 1977, Phys. Rev. A, 16, 986.

Hamilton, A. J. S., Sarazin, C. L., and Chevalier, R. A. 1983, Ap. J. Suppl., 51, 115.

Holt, S. S., Mushotzky, R. F., Becker, R. H., Boldt, E. A., Serlemitsos, P. J., Szymkowiak, A. E., and White, N. E. 1980, Ap. J. (Letters), 241, L13.

Huebner, W. F., Argo, M. F., and Ohlsen, L. D. 1978, J. Quant. Spectrosc. Rad. Transf., 19, 93.

TIMOTHY R. KALLMAN: NASA/Goddard Space Flight Center, Code 665, Greenbelt, MD 20771

JULIAN H. KROLIK: Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138