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PHOTOELECTRIC ABSORPTION CROSS SECTIONS WITH VARIABLE ABUNDANCES

MONIKA BAŁUCIŃSKA-CHURCH
School of Physics and Space Research, University of Birmingham, Birmingham, B15 2TT, England UK

AND

DAN MCCAMMON
Physics Department, University of Wisconsin, Madison, WI 53706
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ABSTRACT

Polynomial fit coefficients have been obtained for the energy dependences of the photoelectric absorption cross sections of 17 astrophysically important elements. These results allow the calculation of X-ray absorption in the energy range 0.03–10 keV in material with noncosmic abundances.

Subject headings: atomic data — X-rays: general

1. INTRODUCTION

The most recent compilation of interstellar photoelectric absorption cross sections used in X-ray astronomy is that of Morrison & McCammon (1983, hereafter MM). This was based on the X-ray cross sections of Henke et al. (1982), together with the review of solar abundance data of Anders & Ebihara (1982). Since the cross sections of the individual elements were added before a numerical fit was made to the energy dependence, it was not possible to vary the relative abundances.

Recent improvements in the spectral resolution of soft X-ray astronomy instruments will allow the study of deviations from the standard cosmic abundances of the material causing photoelectric absorption. Moreover, the cosmic abundances of MM are applicable primarily to the local interstellar medium. There is evidence for deviations from these abundances in the Galaxy as well as in extragalactic sources. Shaver et al. (1983) show that there is a radial abundance gradient in the Galaxy of ~16% per kiloparsec for elements heavier than helium.

Hatsukade (1989; see Koyama 1990) summarizes the evidence that in galaxy clusters the abundance of iron determined for the cluster as a whole has a value between 0.2 and 0.5 of the solar value. Earlier results (Mushotzky 1984) as discussed by Sarazin (1986) generally support the abundance being less than solar. In contrast to this, in elliptical galaxies it is believed that the iron abundance may be 4–10 times greater than the solar value (Sarazin & Wise 1990).

The aim or our work is to provide convenient fits to the photoelectric absorption cross sections for each of 17 elements separately, so that spectral modeling can be performed with an absorption term containing the abundances of some or all of the elements as adjustable parameters.

2. DATA FITTING

The atomic absorption cross sections were taken as in the previous work (MM) from Henke et al. (1982). Polynomial fits have been made to the atomic absorption cross sections in the energy range of 0.03–10 keV for 17 elements: hydrogen, helium, carbon, nitrogen, oxygen, neon, sodium, magnesium, aluminium, silicon, sulphur, chlorine, argon, calcium, chromium, iron, and nickel. In the case of elements with only the K-edge in this energy range, polynomial fits were made each side of the edge; with the L-edge also present three fits were made. Polynomials of up to degree 8 were required. The functions fit Henke's data points with a typical error of 2% and a maximum error of 7%, except for points below 40 eV for argon, calcium, and sodium, where the errors are larger.

The effective cross section per hydrogen atom for a particular set of elemental abundances may be simply calculated from the individual cross sections. Using these functions with the relative abundances assumed in MM should in principle give identical results to the MM polynomial, since the same atomic cross sections were used, and they in fact agree to within 3% below 0.4 keV and to within 1% for the rest of the energy range.

We have incorporated the polynomial fits for each of the 17 elements covering the energy range 0.03–10 keV into FORTRAN subroutines. The FORTRAN source code for these routines, and for a master function that returns the net cross section per hydrogen atom at any energy given a set of relative abundances, is available from NASA's National Space Science Data Center or from the authors (see the Appendix for details).

3. LIMITATIONS

These cross sections are intended to be for the neutral atomic form of the elements and do not take into account the possibility of ionization or the inclusion of material into molecules or grains. None of these has a very large effect on the total absorption (except in the case of complete ionization: see Krolik & Kallman 1984), but hiding a large part of the hydrogen in molecular or ionized form can introduce major errors when measurements of atomic hydrogen column densities are used to estimate total mass. We point out in particular that up to half the hydrogen in the galactic plane may be in molecular form, and up to half at high latitudes may be ionized (Reynolds 1989; see also discussion in Jahoda, Lockman, & McCammon 1990). For interstellar absorption, at least, the small shifts in absorption edge energies with ionization are potentially more interesting than the changes in magnitude of the cross section, since high-resolution spectroscopy should make it possible to use these shifts as diagnostics of the ionization state (Daltabuit & Cox 1972). Compton scattering becomes important above 4 keV and dominates above 10 keV in neutral material. In highly ionized gas it can be important at much lower energies. See

MM and references therein for a more complete discussion of these issues.

Recently Gould & Jung (1991; Jung & Gould 1992) have published calculations of K- and L-shell photoelectric absorption. They point out that, except for noble gases, the experimental data used by Henke are for molecular or solid forms of the elements. The calculations for the atomic form show small decreases in cross section just above the absorption edges, and slightly higher edge energies, particularly for the lighter elements. For oxygen, as the most important example, the K-edge energy is higher by 2.6%, and the cross section just above the K-edge is smaller by ∼16%. The difference decreases to ∼5% at ∼0.7 keV. The relatively small differences in cross section are less likely to be important than the shifts in edge energy, for the reasons given above.

Gould & Jung's procedures also seem to offer the possibility of relatively simple calculation of accurate cross sections and edge energies for arbitrary ionization states. Such data are needed for precise modeling of radiative transfer in highly ionized media (Krolik & Kallman 1984).

Part of the analysis was carried out (by M. B. C.) at the University of Birmingham using the facilities of the SERC *Starlink* node. D. M. thanks Andy Stephan for his assistance in verifying the subroutines. This work was supported in part by NASA grant NAG5-679.

APPENDIX

A set of routines has been written in generic FORTRAN-77 to implement these polynomial fits. The file XSCTNS.FOR contains 17 REAL functions, that will return the photoelectric cross sections for H, He, C, N, O, Ne, Na, Mg, Al, Si, S, Cl, A, Ca, Cr, Fe, and Ni in $\mathrm{cm}^2\ \mathrm{g}^{-1}$, given the photon energy in electron volts. The file TOTLXS.FOR contains a single function that returns the effective cross section in cm^2 per H atom, given the photon energy in electron volts and a set of 17 relative abundances in $\log_{10}$. If standard abundances (as assumed by Morrison & McCammon) are to be used, the file SIGISM.FOR contains a function implementing the MM polynomials that also returns the effective photoelectric cross section in cm^2 per H atom, given the photon energy in electron volts. It executes much faster than TOTLXS, but gives the same results as TOTLXS called with MM relative abundances. All of these routines are valid only over the photon energy range 30–10,000 eV.

These files are available as data set GX-11F, "Cross Sections for 17 Elements," on-line or on floppy disk or magnetic tape from NASA's National Space Science Data Center. To place a request for the magnetic media or to get instructions for retrieving the files on-line, contact NCF::REQUEST (Decnet); REQUEST@nssdca.gsfc.nasa.gov (Internet); National Space Science Data Center–Request Coordination, NASA/GSFC/NSSDC, Code 933, Greenbelt, MD 20771 (mail); (301) 286-6695 (phone); or (301) 286-4952 (FAX). Alternatively, the files are available directly from the authors: 19775::MBC (Decnet); MBC@uk.ac.bham.sr.star (Janet); 47413::McCammon (Decnet); McCammon%wisp.decnet@vms.macc.wisc.edu (Internet).

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