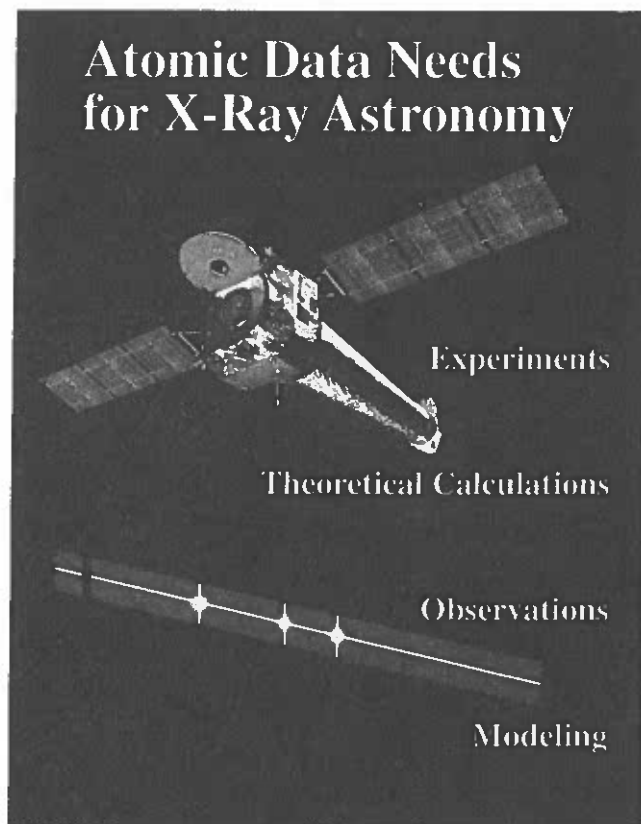




## Atomic Data Needs for X-ray Astronomy

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# Photoionization and Recombination

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**Abstract.** Theoretically self-consistent calculations for photoionization and ( $e + \text{ion}$ ) recombination are described. The same eigenfunction expansion for the ion is employed in coupled channel calculations for both processes, thus ensuring consistency between cross sections and rates. The theoretical treatment of ( $e + \text{ion}$ ) recombination subsumes both the non-resonant recombination ("radiative recombination"), and the resonant recombination ("di-electronic recombination") processes in a unified scheme. In addition to the total, unified recombination rates, level-specific recombination rates and photoionization cross sections are obtained for a large number of atomic levels. Both relativistic Breit-Pauli, and non-relativistic LS coupling, calculations are carried out in the close coupling approximation using the R-matrix method. Although the calculations are computationally intensive, they yield nearly all photoionization and recombination parameters needed for astrophysical photoionization models with higher precision than hitherto possible, estimated at about 10-20% from comparison with experimentally available data (including experimentally derived DR rates). Results are electronically available for over 40 atoms and ions. Photoionization and recombination of He-, and Li-like C and Fe are described for X-ray modeling. The unified method yields total and complete ( $e + \text{ion}$ ) recombination rate coefficients, that can not otherwise be obtained theoretically or experimentally.

## 1. Introduction

Although photoionization and recombination are direct opposite processes as they occur in nature, they are usually treated in independent theoretical frameworks. This basic inconsistency, directly related to ionization balance in radiatively ionized media, and consequent inaccuracies, propagate through the photoionization models employed in astrophysics. A further division, largely artificial, is made in theoretical methods used to compute electron-ion recombination rates. Two sets of data are usually calculated: (i) "radiative recombination" (RR), calculated using background, or non-resonant, photoionization cross sections, and (ii) "di-electronic recombination" (DR) representing the contribution of autoionizing resonances, first shown to be important by Burgess (1964). That this procedure is not only theoretically unsatisfactory, but also impractical in most cases, as seen from both theoretical calculations and experimental measurements of photoionization and recombination cross sections. The simple reason is that the resonances are inseparable from the background. The cross sections contain, in general, extensive and interacting Rydberg series of resonances; the non-resonant and resonant contributions are not accurately separable (except, possibly, for few-electron, highly charged ions). The large number of photoionization cross sections computed under the Opacity Project exhibit these features in detail (*The Opacity Project Team* 1995, 1996 - compiled publications and data). In addition, the cross sections for photoionization and recombination of excited states, particularly metastable levels, may contain even more complicated resonances than the ground state (Luo et al. 1990). Experimentally, of course, the measurements always yield a combined (RR + DR) cross section (albeit in limited energy ranges usually accessible in experimental devices).

Therefore a theoretical method that accounts for both the resonant and the non-resonant recombination in a unified manner is desirable, and has been developed (e.g. Nahar and Pradhan 1994, Zhang et al. 1999), based on the close coupling (CC) approximation using the R-matrix method (Burke and Seaton 1984, Berrington et al. 1987, Hummer et al. 1993) as used in the Opacity Project and the Iron Project (hereafter OP and IP). Photoionization cross sections may be computed essentially for all bound