Charge Transfer Calculations and Database for Astrophysics

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Abstract

A variety of theoretical approaches, having different but overlapping energy ranges of applicability, are applied to investigate charge transfer processes for collisions of atomic ions with atoms and molecules. The methods include quantal molecular-orbital close-coupling, classical trajectory Monte Carlo, and continuum distorted wave methods. Recent collision systems studied include S^{4+} + H, S^{4+} + He, N^{7+} + He, H_2O, CO, and CO_2, $O^{q+}(q = 1-8)$ + H, H_2, and $S^{q+}(q = 1-16)$ + H_2. The database effort is concentrating on astrophysically important reactions of atomic ions X^{q+}(X=H–Zn, q=1–4, and selected higher charges) with H, He, various metal atoms, H_2, and other selected molecular targets. Existing data, much of it produced by us, have been compiled and critically evaluated. Data for many reactions missing in the literature are estimated using the multichannel Landau-Zener approximation. Fits to cross sections and rate coefficients using standard functions are provided as well as tabulations of the raw data. The database is available on the World Wide Web at **cfadc.phy.ornl.gov/astro/ps/data**.

1. Introduction

Charge transfer, occuring in a very large range of astrophysical environments, can be decisive in establishing ionization structure, energy transfer, and inducing IR to x-ray radiative relaxation. However, little comprehensive data exist for complex projectile ions or targets more complex than atomic hydrogen. Therefore, to aid in the remediation of this situation, we are engaged in two efforts: (i) the calculation of charge transfer cross sections and rate coefficients using a variety of modern theoretical methods and (ii) the development of an on-line database of charge transfer reactions.

2. Theoretical Methods

To perform calculations for charge transfer, we use a variety of theoretical methods. Each method has its own advantages as well as disadvantages which can be classified according to the nature of the projectile ion and neutral target, the relevant energy range, the type and number of channels, and the degree of computational difficulty. For low-energy collisions, we employ the quantal molecular-orbital close-coupling (QMOCC) method. Radial, and often rotational, couplings are included in our QMOCC approach. For molecular targets, orientation and vibrational excitation of the target are also considered. The classical trajectory Monte

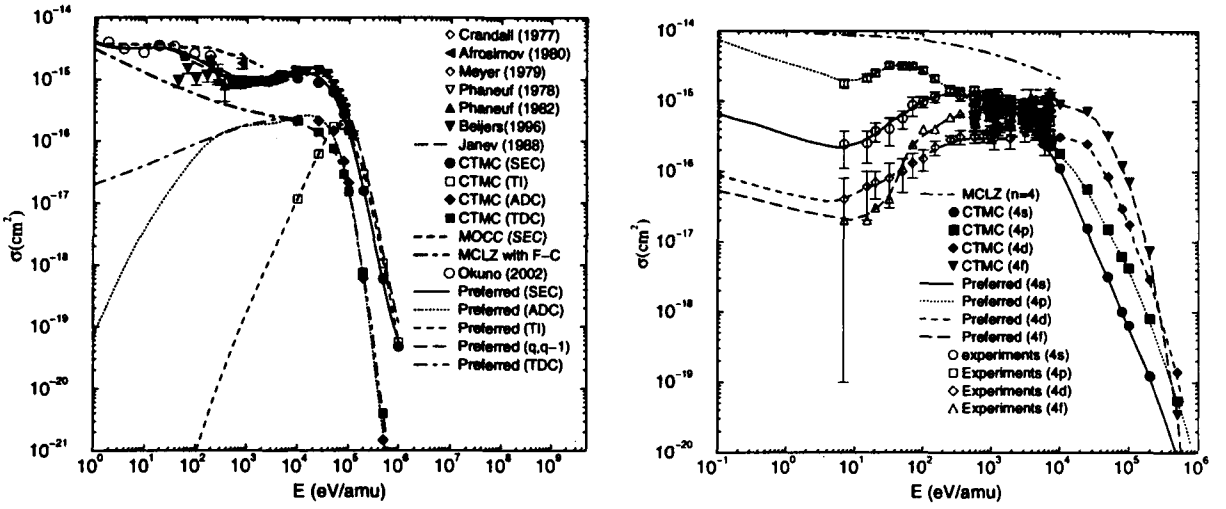

Fig. 1.— (a) Total cross sections for $O^{3+} + H_2$. (b) SEC state-selective cross sections for $O^{6+} + H_2$.

Carlo (CTMC) method is applied to collision problems at intermediate energies. For multi-electron targets such as He and H_2, CTMC has the advantage of providing data, in addition to single-electron capture (SEC), on multielectron processes such as true double-electron capture (TDC), transfer ionization (TI), and double-electron capture followed by autoionization (ADC). For relatively high collision energies, the continuum distorted wave (CDW) method can be used, but we apply it only for SEC calculations. A method which has been routinely used for astrophysical applications is the Landau-Zener (LZ) aproach. We use a multichannel (MCLZ) variant and for molecular targets, Frank-Condon ionization factors are used to treat the vibrational states of the product ion for SEC. We have also developed a method to treat total double capture (the sum of ADC and TDC) with the MCLZ approach.

3. Database

For our database effort, we i) collect existing experimental and theoretical data from the literature, ii) where data for a reaction is missing from the literature, cross sections and rate coefficients are computed using one or more of the methods described above, iii) all data are compiled and evaluated, and iv) the resulting preferred cross sections and rate coefficients are fit to standard functions (e.g. Chebychev polynomials).

4. Representative Results

A number of individual calculations have been completed as well as compilations and fittings for a series of collision systems. For example, for $O^{q+}(q = 1 - 8) + H_2$, we considered charge transfer for all accessible final states with $n \leq 10$ for all four possible channels (SEC, TDC, TI, and ADC), which gives: 32 total, about 320 n-selective, and about 1760 n, l-selective cross sections. The cross sections were obtained and fitted over a large energy range from at least 1 eV/u to 10 MeV/u. A few examples are shown in figures 1-3. All of the results will be available on the ORNL/UGA Charge Transfer Database for Astrophysics.

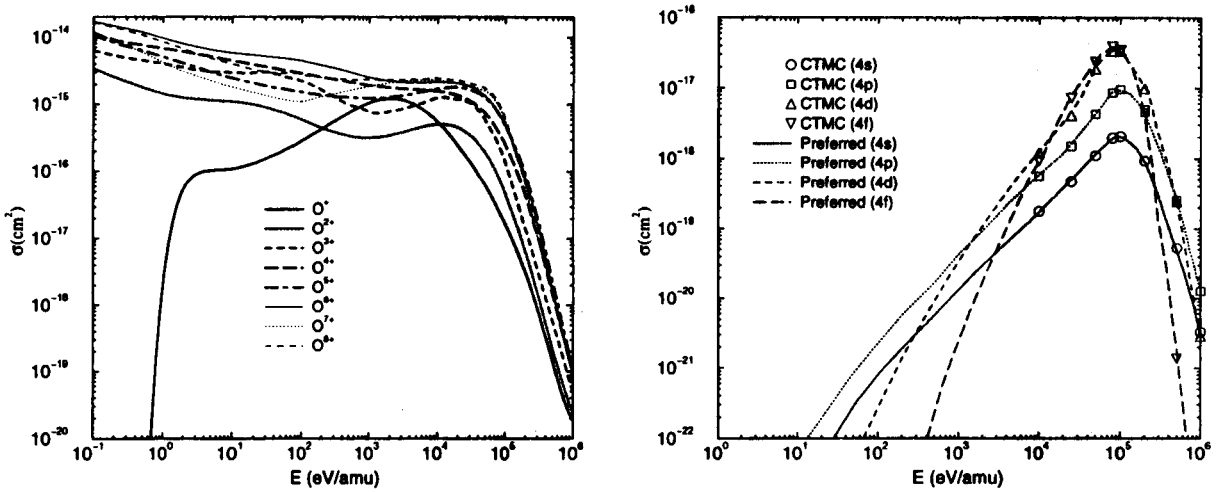

Fig. 2.— (a) The preferred total SEC cross sections for $O^{q+}(q = 1-8) + H_2$. (b) TI state-selective cross sections for $O^{5+} + H_2$

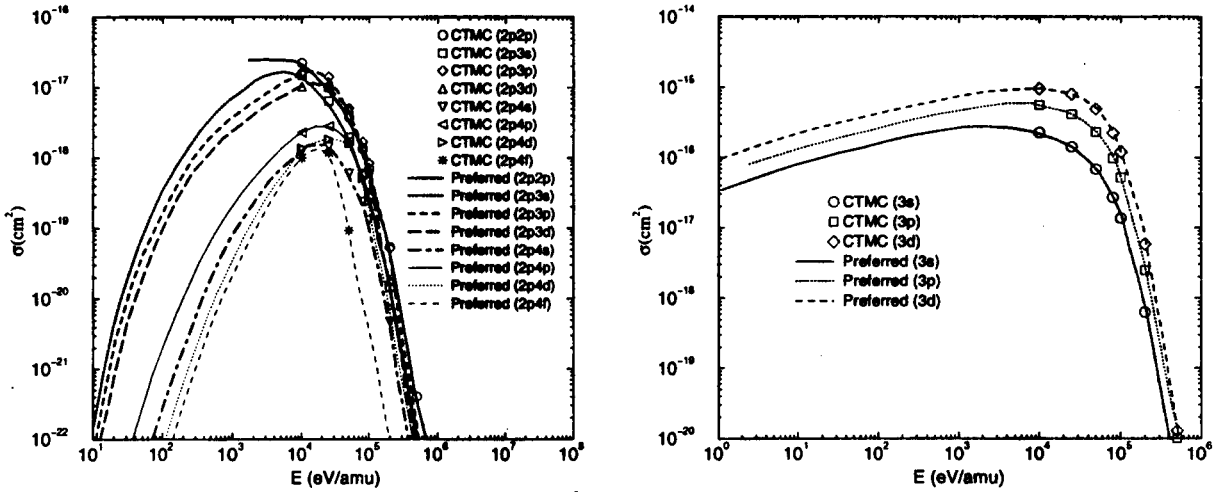

Fig. 3.— TDC state-selective cross sections for $O^{2+} + H_2$. ADC state-selective cross sections for $O^{7+} + H_2$.

Acknowledgments

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