Final Report
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Ultraviolet and Visible Emission Mechanisms in Astrophysics

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This final report summarizes the work accomplished for the entire period of the award, January 1, 1999 to January 31, 2003. For the first year (1999), the project was located at Oak Ridge National Laboratory (NRA-98-03-UVG-026), but was relocated with the PI to the University of Georgia for the remainder of the grant period. When the project was at ORNL, the budget primarily supported the PI's salary. With the relocation to UGA, the budget was rewritten to fund a postdoctoral associate. A search for the postdoc began in October 1999, but the most suitable candidate (Dr. Jianguo Wang) was not able to arrive until June 1, 2000. For the final two years of the project at UGA, the award period was February 1, 2000 to January 31, 2002. Due to the late arrival of Dr. Wang, a one year no-cost extension was requested and granted, extending the grant to January 31, 2003.

The project involved the study of ultraviolet (UV) and visible emission mechanisms in astrophysical and atmospheric environments. In many situations, the emission is a direct consequence of a charge transferring collision of an ion with a neutral with capture of an electron to an excited state of the product ion. The process is also important in establishing the ionization and thermal balance of an astrophysical plasma. As little of the necessary collision data are available, the main thrust of the project was the calculation of total and state-selective charge transfer cross sections and rate coefficients for a very large number of collision systems. The data was computed using modern explicit techniques including the molecular-orbital close-coupling (MOCC), classical trajectory Monte Carlo (CTMC), and continuum distorted wave (CDW) methods. Estimates were also made in some instances using the multichannel Landau-Zener (MCLZ) and classical over-the-barrier (COB) models. Much of the data which has been computed has been formatted for

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inclusion in a charge transfer database on the World Wide Web (cfadc.phy.ornl.gov/astro/ps/data/). A considerable amount of data has been generated during the lifetime of the grant. Some of it has not been analyzed, but it will be as soon as possible, the data placed on our website, and papers ultimately written.

While the MOCC, CTMC, and CDW techniques are well established, we have applied them to complex collision systems and situations which have not been previously well studied. We have therefore made improvements to the theory in an effort to address these issues. For example, the CTMC method has been traditionally applied to fully-stripped projectile ions. To give us the ability to treat projectiles with multiple electrons, we have modified the CTMC approach to account for the screening of the projectile core due to the electrons in the final state binning of charge transfer results. To accomplish this, we have considered two methods: (i) a binding-energy dependent effective charge and (ii) a non-integer shift of the principal quantum number n (the so-called quantum defect). Both methods take into account the non-hydrogenic nature of low-lying (small n) states of the multielectron ions. The method advocated in (ii) was described in Raković et al. (2001) while the effective charge approach was presented in Schultz et al. (2001) with detailed comparisons to the quantum-defect method. Subsequent calculations by our group have used both methods.

We have also extended CTMC to treat more complex multielectron diatomic and triatomic molecular targets, such as H_2O, CO, and CO_2 relevant to, for example, cometary UV/x-ray emission (Hasan et al. 2001). In the method, we (i) incorporate the measured (or calculated) molecular-orbital vertical ionization energies, (ii) account for the electronic radial distribution of the molecular target, and (iii) sum the individual results for both non-bonding and bonding orbitals with an independent-electron model. To test our approach, we have worked closely with the experimental groups at ORNL (Charlie Havener) and at the University of Nevada, Reno (UNR; Rami Ali). The ORNL group has measured single and double total electron capture for S^{5+} and S^{7+} collisions with H_2, CO, H_2O, and CO_2 while the UNR group has measured state-selective single electron capture for N^{7+} and O^{7+} collisions with He, H_2O, CO, and CO_2. We have made CTMC, MCLZ, and COB calculations for most of these reactions with encouraging results. A joint experimental/theoretical paper for the UNR work was presented in Hasan et al. (2001).

MOCC has traditionally been only applied to ion-atom collisions, but in recent years the approach has been extended to ion-molecule collisions. We first applied the MOCC approach to calculate electronic state-selective cross sections in collisions of H^+ with CO (Kimura et al. 2000). Vibrationally resolved cross sections for O^{3+}/H_2 have been completed (Wang et al. 2003b), while for the H^+/CO system they are in preparation (Stancil et al. 2003).

The continuum distorted wave (CDW) approach, which is useful for supplementing the CTMC calculations at high energies, was also primarily developed for hydrogenlike systems. We have ap-

plied it in an adopted formulation to treat multielectron atomic ion projectiles. For low energies, we have also applied MCLZ to supplement the CTMC and MOCC calculations.

CTMC, CDW, and MCLZ calculations for all O^{q+} ions, $q = 1 - 8$, colliding with H have been performed giving total and final state-selective results for single electron capture. Recommended cross sections and rate coefficients, including comparison to existing experimental and theoretical data are now available on our website. An extensive paper describing this work is in prepartion (Wang et al. 2003c), however the techniques used in this comprehensive work was documented in our study of S^{4+}/H (Stancil et al. 2001). CTMC and CDW calculations for all S^{q+} ions, $q = 1 - 16$, colliding with H have also been computed. MCLZ calculation will be performed and the analysis performed for the O^{q+}/H work will be repeated for S.

CTMC calculations for all O^{q+} ions, $q = 1 - 8$, and S^{q+} ions, $q = 1 - 16$, colliding with H_2 for single electron capture (SEC), true double electron capture (TDC), transfer ionization (TI), and autoionization following double capture (ADC) have been completed. Due to the two-electron nature of the double electron capture processes (TDC and ADC), the determination of their cross sections also required knowledge of the branching ratios for radiative decay and autoionization of the doubly-excited two-electron capture states. The branching ratios were calculated for all O and S ions using the code AUTOSTRUCTURE. The details of the methods used are described in our study of the S^{4+}/He system (Wang et al. 2002). Fits to the cross sections are available on our website which also include MCLZ for SEC. The fits are currently being used by modelers of UV/x-ray emission from Jupiter. Manuscripts describing the charge transfer calculations are in preparation (Raković et al. 2003a,b). MCLZ calculations for O^{q+}, $q = 2 - 8$ and CDW of O^{8+} and S^{16+} with He have also been performed.

An invited review article was written for a meeting at the University of Kentucky on photoionized plasmas which discussed the various theoretical methods used to compute charge transfer cross sections, sources of charge transfer data, and ways to estimate a charge transfer cross section if data are lacking (Stancil 2001). Two invited review articles were also written which described the progress in using the MOCC method (Cooper et al. 2001, 2002).

A review article on the status of charge transfer calculations relevant to cometary UV/x-ray emission was written for the International Conference on Atomic and Molecular Data and Its Applications (ICAMDATA) (Stancil et al. 2002). The article also reported preliminary results for modeling the experimental UV/x-ray emission cascade spectra of Ne^{9+} following Ne^{10+} collisions with He as measured at UNR by Rami Ali. The model spectra used CTMC and MCLZ SEC calculations. X-ray spectra resulting from collisions of Si^{13+}, S^{15+}, and Ar^{17+} with various neutral atom and molecules were measured at Kansas State Univ. (Tawara et al. 2001b) and will be modeled with future charge transfer calculations.

Wang & Stancil (2002) performed a survey of all experimental and theoretical data available for H^+/H_2 for all isotope (D, T) substitutions. They provided recommended fits of cross sections and rate coefficients which are available on our website. As a service to the photoionization modeling community, and having the code CLOUDY in mind, MCLZ SEC calculations of total and state-selective cross sections and rate coefficients for all ions from Li to Zn for charges $q = 2 - 4$ colliding with He were computed for collisions systems which lacked data (about 75%). All total rate coefficients and many of the state-selective results have been fitted and placed on our website. In addition, total rate coefficients were estimated for Si/He^+ and Fe/H^+ following the request of the CLOUDY author Gary Ferland. Once this large amount of data is checked, a manuscript will be submitted (Wang et al. 2003f), but for now it is available for the community's use, with caution.

Finally to summarize, cross sections for the following individual collision systems have been calculated with the follow manuscripts published: O^+/H and H^+/O (Stancil et al. 1999, MOCC, CTMC, CDW), Si^{2+}/He (Suzuki et al. 1999, MOCC), H^+/CO (Kimura et al. 2000, MOCC), N^{7+}/H and Cl^{7+}/H (Thompson et al. 2000, MOCC, MCLZ, experiment), N^{2+}/He (Cooper et al. 2001, MOCC), Si^{4+}/He (Suzuki et al. 2001a,b, MOCC), $Si^{(3-5)+}/He$ (Tawara et al. 2001a, experiment, MCLZ), S^{4+}/H (Stancil et al. 2001, MOCC, CTMC, CDW, MCLZ), S^{4+}/He (Wang et al. 2002, MOCC, CTMC, CDW, MCLZ), O^{3+}/H (Wang et al. 2003a, MOCC, MCLZ). The following papers are in press: Ne^{2+}/He (Imai et al. 2003a, MOCC) and B^{2+}/H (Turner et al. 2003, MOCC) and the following are in preparation: O^{3+}/H_2 (Wang et al. 2003b, MOCC), H^+/CO (Stancil et al. 2003, MOCC, CTMC, CDW), S^{2+}/He (Imai et al. 2003b, MOCC), B^{2+}/H (Wang et al. 2003d, MOCC, CTMC, CDW), and Ne^{2+}/He (Wang et al. 2003e, MOCC, radiative CX, CTMC, CDW).

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