Charge Transfer Calculations and Database for Astrophysics

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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.

To investigate charge transfer, we apply a number of very diverse theoretical approaches that have different but overlapping energy ranges of applicability. These 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, and N^{7+} + He, H_2O, CO, and CO_2. An extensive set of calculations on all O and S ions colliding with H_2 is in progress.

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 theoretical and experimental cross section and and rate coefficient data, much of it produced by us, have been compiled and critically evaluated. Data for many reactions missing in the literature are being estimated utilizing nonadiabatic models (e.g. multichannel Landau-Zener). 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 **www-cfadc.phy.ornl.gov/astro/ps/data/**.

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