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**Atomic and Molecular Physics and Data Activities for Astrophysics at Oak Ridge National Laboratory**

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— I'm honorary first author. Dave Schultz wrote it all before I knew of it.

**Abstract:** The atomic astrophysics group at ORNL produces, collects, evaluates, and disseminates atomic and molecular data relevant to astrophysics and actively models various astrophysical environments utilizing this information. With the advent of the World Wide Web, these data are also being placed on-line to facilitate their use by end-users. In this brief report, the group's recent activities in data production and in modeling are highlighted. For example, we describe recent calculations of elastic and transport cross sections relevant to ionospheric and heliospheric studies, charge transfer between metal ions and metal atoms and novel supernova nebular spectra modeling, ion-molecule collision data relevant to planetary atmospheres and comets, and data for early universe modeling.

**I. Introduction**

The atomic astrophysics group at Oak Ridge National Laboratory (ORNL) is involved in the study of a wide range of astrophysical environments including the Jovian aurora and dayglow, Type Ia supernovae, molecule production and destruction in supernovae, and pre-galactic chemistry. This work is supported by active theoretical production of data describing collisions among ions, atoms, and molecules over a wide range of energies and reactions channels. Furthermore, these activities are coordinated with other astrophysical research at ORNL including experimental groups which investigate electron and ion collisions with ions, atoms, molecules, and surfaces, an atomic data center, and experimental and theoretical nuclear astrophysics programs involving radioactive beams, Type II supernova explosion modeling, and nuclear reaction network calculations and measurements.

**II. Jovian auroral x-ray emission and dayglow**

Auroral x-ray emission from Jupiter was observed by the *Einstein* satellite and recently by *ROSAT*. Clues to the origin of these emissions are given by the detection by the *Voyager* spacecrafts and the recent *Ulysses* flyby of energetic Iogenic oxygen and sulfur ions diffusively impinging into Jupiter's atmosphere. These measurements lead Cravens and coworkers (Horanyi et al. 1988, Cravens et al. 1995) to suggest that the x-rays are produced by radiative decay from highly excited states created by charge transfer in collisions of the precipitating O and S ions with the principal atmospheric constituent, H<sub>2</sub>.

Existing broad-band *ROSAT* measurements of the x-ray spectra do not allow for a detailed examination of the lines and/or continuum distribution, but new missions such as *AXAF* will almost certainly provide more strenuous tests for predictions of this emission. In fact, the early models suffer from the lack of a complete and assessed database of relevant atomic and molecular reaction cross sections. Thus, we are in the process of producing

the required state-selective charge transfer cross sections for all O and S ions with H, H<sub>2</sub> and He. This database will provide realistic  $n, l$  state distributions to form the basis for cascade/radiative decay simulations. Notably, distinction between H and H<sub>2</sub> is crucial as the excited state distributions and cross section magnitudes differing greatly. In addition, we will provide other inelastic cross sections and distributions such as those relevant to ionization and excitation. These data will be used to model the x-ray spectra, and diagnose properties of the Jovian atmosphere such as UV emission from excited H<sub>2</sub> and the range and straggling of ions.

Also detected since the *Voyager* missions, investigation of the Jovian dayglow continues to be an active area of investigation by our group. Models (e.g. Liu and Dalgarno 1996) of this ultraviolet emission from ro-vibronic de-excitation of solar radiation bombarded molecular hydrogen are being improved and new atomic and molecular data incorporated. Correlations with solar cycle of the dayglow and temperature and density profiles of the Jovian atmosphere are subjects of these ongoing investigations.

### III. Cometary x-ray emission

The unexpected observation of x-ray emission from comet Hyakutake by Lisse and coworkers (Lisse et al. 1996) and subsequently from more recent comets and in archival data, has stimulated speculation as to the mechanism producing these x-rays, and as to what these emissions can tell us about comets. Though a number of models based, for example, on scattering of solar x-rays, have been put forward to account for these observations, the most likely mechanism seems to be radiative decay similar to that described for the precipitating heavy ions in Jupiter's atmosphere. In the cometary case, the ions are of solar wind origins (e.g. C, O, Ne, Fe) and the neutrals are comet gas species such as H<sub>2</sub>O, OH, O, H, and CO. In addition, the ion energies typical of the solar wind are lower than those accelerated by the Jovian magnetosphere. As in the Jovian x-ray case, models (e.g. Häberli et al. 1997) have been hampered by the lack of state-selective charge transfer data for the relevant ion-neutral pairs and other inelastic data needed for ionization balance and transport simulations. Also, next-generation x-ray astronomy satellites will allow much higher resolution observations, so we are constructing realistic models to compute the needed database of reaction rates and will obtain resulting synthetic spectra to potentially improve the present understanding of this emission, and of cometary dynamics and chemistry.

### IV. SNe Ia nebular spectra: atomic data and new constraints on explosion models

Though SNe Ia are important generators of heavy elements and observations of SNe Ia have recently been exploited to place new limits on the cosmological parameters relating to the mass density, expansion rate, and cosmological constant, largely due to the relative uniformity of their photospheric-phase light curves, no SNe Ia progenitor has been identified and there is still considerable debate as to the explosion mechanism and heavy element yields. Thus, we have undertaken to try to constrain these open variables by performing nebular spectra synthesis based on the best available atomic data. In fact, the ionization balance in the ejecta of a SN is strongly affected by charge transfer, even though to this point, this

important reaction channel has been neglected in modeling. Further, since Ia's are deficient in H and He, the relevant charge transfer is between iron-group ions and neutrals, data for which were previously lacking.

Thus, we have performed basic calculations of these new charge transfer rates, and utilized new electron impact inelastic rates to obtain synthetic spectra for several well observed SNe Ia's. The results (e.g. Liu et al. 1997, Liu et al. 1998) reflect the importance of this more complete accounting of the atomic processes, and has, in fact, resulted in a favoring of sub-Chandrasekhar (SC) mass progenitors. This conclusion is based on the improved modeling of the nebular spectra for SC models and predicts, as well, significantly different ionization and thermal structures than obtained with Chandrasekhar mass models. This work is continuing by refinement of the first charge transfer calculations for the complex metal-metal collisions (Krstić et al. 1998), and by exploring elaborations of the spectrum modeling to extend to earlier and later epochs.

## V. Elastic and related transport cross sections

The elastic scattering of particles in weakly ionized plasmas leads to momentum transfer often affecting the transport properties of these environments. This process influences, for example, ionospheric and exospheric coupling and exospheric escape of hydrogen influenced by momentum transfer in the upper atmosphere of earth or other planets. Also, the interaction of interstellar hydrogen with solar wind protons in the outer heliosphere is in part determined by elastic scattering accounting for the solar wind termination shock and heliopause. However, no work exists extensively tabulating the elastic differential cross section, especially over a wide range of energies, for such collision pairs of high importance for astrophysics as  $H^+ + H$ ,  $H^+ + H_2$ ,  $H + H$ ,  $H + H_2$ , and  $H^+ + He$ , so we have produced a large volume of this data and provided fits to the differential cross section, constrained to match the total elastic cross section and its moments (diffusion and viscosity) upon integration over scattering angles, to be published in 1998 and made available over the WWW (Krstić and Schultz 1998). This work contains fits to over 1500 elastic cross sections and follows earlier classical (Bachmann 1993) and fully quantal tabulations (Schultz et al. 1995) for much smaller subsets of collisions.

## VI. Pre-galactic chemistry

Chemistry began in the postrecombination era of the early Universe after the formation of the first neutral atoms. Due to the extreme conditions of uniform low density, intense background radiation, absence of dust grains, and a limited set of light elements and isotopes (H, D,  $^4He$ ,  $^3He$ , and Li), the molecular fraction of the primordial gas never exceeded  $\sim 10^{-6}$ . A comprehensive database of the important gas-phase reactions has been assembled and utilized in a nonequilibrium chemical model to track the production of primordial molecules (Stancil et al. 1996, 1998) in the early expanding Universe. The chemistry is generally complete except that some uncertainty remains in the abundance of  $H_2$  due to limited information on its formation via charge transfer of  $H_2^+$  with H. As the Universe continued to expand, density perturbations in the otherwise uniform flow collapsed to form the

first distinct cosmological objects. The size of these objects and their ability to continue to contract, possibly to stellar densities, is controlled by the gas' ability to remove heat produced in the gravitational collapse. This cooling is, however, provided by the small, but crucial, molecular fraction (Tegmark et al. 1997). The early Universe database is currently being extended to include relevant reactions and molecular cooling functions. Models will be constructed to investigate the formation of these early objects under various hydrodynamic collapse scenarios.

## VII. Atomic and molecular data center activities and resources

Certainly, the vast majority of the information we obtain remotely about the universe comes from light emitted by atoms and molecules. As illustrated in this brief report of our recent activities, a large amount of atomic and molecular collision data is required to provide models and interpretations of astrophysical phenomena, only a fraction of which already exists. To aid in the collection of such data, and to serve the community by evaluating and disseminating this information, a data center was established at ORNL in 1958, originally to support the development of controlled fusion energy. Our efforts in astrophysics are aided by the resources available through the data center, such as its categorized on-line bibliography, various evaluated databases, participation in an international network of similar data centers, and a closely associated atomic and molecular collisions experimental group. Much of the data available from these sources is provided through a new WWW site ([www-cfadc.phy.ornl.gov](http://www-cfadc.phy.ornl.gov)). The data will in the future continue to be augmented and improved, and the end-user's ability to search, display, and download data refined. These efforts will lead to a significant resource for the astrophysics community.

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