J. Andersen (ed.), Reports on Astronomy, Vol. XXIVA, 1–20.

COMMISSION 14: ATOMIC AND MOLECULAR DATA[1]

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In recognition of its special interdisciplinary character, IAU Commission 14 is linked directly to the Executive Committee. The Commission's role is to inform the astronomical community of new developments in the diverse fields of research which involve atoms and molecules. Conversely it endeavours to sensitize the research community active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commision 14 tries to foster long term relations and collaborations between the two communities and, when necessary, to alert funding authorities to the specific needs of ground and space based astronomy for specific atomic and molecular data.

This report is one of the main contributions of Commission 14 to the information of the astronomical community. Several meetings concerned, at least in part, with the need and availability of atomic and molecular data for astrophysics were also sponsored or co-sponsored. In the last triennium, Commission 14 cosponsored IAU Symposium 194 "Astrochemistry: From Molecular Cloud to Planetary Systems" held in Sogwipo (Korea) from Aug. 23 to 27, 1999 and organized by Commission 34. A Joint Discussion: JD1 on "Atomic and Molecular Data for Astrophysics, New Developments, Case Studies and Future Needs" has been planned for the XXIVth IAU General Assembly in Manchester (Aug. 7-19, 2000) and cosponsored by Commissions 15, 16, 29, 34, 36, 40 and 44. Several other Joint Discussions to be held at the Manchester General Assembly are co-sponsored by this commission.

The present report comprises six sections established by the specialized Working Groups of Commission 14. It is made available on the Commission 14 Website:
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and its mirror `http://cfa-www.harvard.edu/amp/iau14`.

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[1] Committee of the Executive Committee.

3. WORKING GROUP 3: COLLISION PROCESSES

PRESIDENT: D. R. SCHULTZ
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Within the broad classification "atomic and molecular collision processes" that are of active or anticipated interest in astrophysics, several hundred published works have appeared since the last summary report of this working group in 1996. Owing to the size and scope of this body of work, rather than seeking to comprehensively review it, here we attempt to identify works of particular importance and compilations that make use of the data especially efficient. Also, since a significant overlap between the atomic and molecular collision processes that are relevant to fusion energy development and those relevant to astrophysics exists, a majority of the literature references of interest can be found using the bibliographic search engine at the ORNL Controlled Fusion Atomic Data Center (CFADC 1999) which currently covers the period 1978 to present. Categorized bibliographies based largely on this database dating from 1969 to 1998 have also been published (CIAMDA 1998). For ease of organization, here we sub-divide "collision processes" using the following scheme: (1) electron impact of atoms and ions, (2) electron impact of molecules, (3) ion-atom and atom-atom collisions, (4) ion-molecule and atom-molecule collisions, and (5) reactive scattering and chemistry. Each of these sub-classes contains the pertinent range of collisions processes (e.g. elastic scattering, excitation, ionization, recombination, particle interchange, *etc.*).

3.1. Electron Impact of Atoms and Ions

Electron collisions with atoms and ions constitute the major excitation mechanism in the majority of astrophysical environments from the solar corona, to planetary nebulae, to active galactic nuclei, and therefore has seen significant activity over the report period. A nearly comprehensive list of targets studied include He^* (Zhou et al. 1998), Li (Wutte et al. 1997), C (Dunseath et al. 1997; Zhang & Sampson 1997), C^+ (Smith et al. 1996), O (Thomas et al. 1997; Majeed & Strickland 1998), O^+ (McLaughlin & Bell 1998), Ne^{2+} (Ramsbottom & Bell 1998), Mg^{5+} (Ramsbottom & Bell 1997a), Mg^{7+} (Bhatia & Thomas 1998), Al^{10+} (Stancalie et al. 1999), S^+ (Ramsbottom et al. 1996; Liao et al. 1997), S^{2+} (Tayal 1997), Ar^{2+} (Galavis et al. 1998), Ar^{3+} (Ramsbottom & Bell 1997b), Fe (Pelan & Berrington 1997), Fe^{3+} (Zhang & Pradhan 1997), Fe^{10+} (Gupta & Tayal 1999), Fe^{11+} (Binello et al. 1998), Fe^{12+} (Gupta & Tayal 1998), Fe^{14+} (Bhatia et al. 1997; Griffin et al. 1998a), Fe^{15+} (Cornille et al. 1997), Fe^{20+} (Phillips et al. 1996; Zhang & Sampson 1997), Fe^{21+} (Ait-Tahar et al. 1996), Fe^{23+} (Berrington & Tully 1997; D'Cruz & Sarazin 1998), Co^+ (Watts 1998), Co^{2+} (Shaw et al. 1998), Ni^+ (Watts et al. 1996), Ni^{2+} (Watts & Burke 1998), Ni^{4+} (Teng et al. 1998), Ni^{11+} (Matthews et al. 1998), Li-like ions (Safronova et al. 1996; Burgess et al. 1998), F-like ions (Berrington et al. 1998), Na-like ions (Keenan et al. 1996; Kimura et al. 1998), and Al-like ions (Saraph & Storey 1999). Rate coefficients for atoms and ions of H to Ni can be found in Mazzotta et al. (1998). A variety of ions have been studied experimentally with the merged-beamed technique at ORNL with much of the data accessible via the WWW (e.g., Si^{2+}, Wallbank et al. 1997).

Electron-impact ionization of atoms and ions has seen significant advances in theoretical methods particularly involving studies of H targets. These include time-dependent lattice methods (Robicheaux et al. 1997), convergent close-coupling and R-matrix approaches (Scott et al. 1997), and time-dependent close-coupling methods (Pindzola & Robicheaux 1996). Theoretical data on various relevant target species include H^*, Li, O^{5+}, Na, and K (Bray 1996), C^+ (Qian & Pan 1998), Li-like ions (Chen et al. 1996), Na-like ions (Pindzola et al. 1998), and Mg-like, Cu-like, and Zn-like ions (Badnell 1999). A tabulation of analytical ionization rate coefficients for all atoms and ions of H to Ni has been compiled by Voronov (1997) and for all carbon ions by Chang & Ordonez (1998). Majeed & Strickland (1998) have surveyed the data for O and Bannister (1996; see also for other experiments) has measured the ionization cross section for some Ne ions with the ORNL crossed-beam apparatus.

A multitude of data for radiative recombination (RR) and dielectronic recombination can be found on the WWW (Verner et al. 1999; Pindzola et al. 1999). Specific systems which have been studied recently include Li^{+} (Zavodszky et al. 1998), all C ions (Nahar & Pradhan 1997; Safronova & Kato 1996, 1998), all N ions (Nahar & Pradhan 1997), all O ions (Nahar 1999), Ne^{2+} (Kisielius et al. 1998), Ne^{7+} (Zong et al. 1998), many Fe ions (Nahar et al. 1997, 1998; Moribayashi et al. 1997; Nahar & Bautista 1999), Fe^{21+} (Chen et al. 1998), Fe^{24+} (Gorczyca & Badnell 1997), C-like ions (Nahar 1996), F-like and Ne-like ions (Jacquemot et al. 1998). However, in recent years three issues have arisen which may call into question the reliability of theoretical electron-ion recombination data or its use in particular environments. In the former instance it has been argued by Badnell et al. (1998) that the neglect of radiation damping effects on low-energy resonances can result in a significant overestimation of RR rate coefficients. On the other hand, at very low energies, experiments (Gao et al. 1997) on ion storage rings have measured RR rate coefficients which are much larger than suggested by theory. Measurements of dielectronic recombination in well-defined electric fields find an enhancement which should be important in astrophysical environments except those with an extremely low ionization fraction (Savin et al. 1996). Some calculations in electric fields have been performed by Griffin et al. (1998b).

Elastic collisions between electrons and atoms/ions can be crucial in determining the transport properties of electrons in plasmas/gases and so we note several recent works on elastic electron scattering: He (Fursa and Bray 1997), N^{1-6+} (Greenwood & Williams 1997), and O (Agrawal & Baluja 1996). Mayol & Salvat (1997) have given a tabulation for all neutral atoms of H through U.

3.2. Electron Impact of Molecules

Electron collisional excitation of molecules is an important process in many plasma environments including planetary atmospheres and high-excitation nebulae. It can play a significant role in line excitation and cooling when energetic electrons are available, i.e. photo-electrons. Recent studies of rotational excitation include H_2 (Danby et al. 1996), HeH^{+} and NO^{+} (Rabadán et al. 1998), CO (Randell et al. 1996), O_2 (Mukherjee & Ghosh 1996), H_2O (Gianturco et al. 1998a), O_3 (Gianturco et al 1998b), CO_2 (Gianturco & Stoecklin 1997), and SO_2 (Gianturco et al. 1997). Vibrational excitation due to electron collisions has been investigated for H_2 (Lee et al. 1996a; Kazanskii 1996; Mazevet et al. 1998), HD (Kazanskii 1996), N_2 (Grimm-Bosbach et al. 1996; Sweeney & Shyn 1997), OH (Chen & Morgan 1997), CO (Gibson et al. 1996), and CH_4 (Bundschu et al. 1997) while studies of electronic excitation of H_2 (Celiberto et al. 1996), CO (Lee et al. 1996b; Zubek et al. 1997; Zetner et al. 1998), CO, CO_2, and SO_2 (Fomunung et al. 1996), N_2 (Gillan et al. 1996), NO (Mojarrabi et al. 1996), O_3 (Sweeney & Shyn 1996), H_2O (Morgan 1998), H_2S (Michelin et al. 1997), and CH_4 and SiH_4 (Bettega et al. 1998) have been performed.

Cross sections have been measured or calculated for ionization of H_2, N_2, O_2, H_2O, and CO_2 (Straub et al. 1996a, 1996b, 1998), H_2 and H_2O (McCarthy 1996); dissociation of H_2O (Kedzierski et al. 1998; Tarnovsky et al. 1998), N_2O (Furuhashi et al. 1997); and dissociation and ionization of H_2 (Celiberto et al. 1997), CO^{+} (Belic et al. 1997), N_2, O_2, CO_2, and CH_4 (Tian & Vidal 1997, 1998a, 1998b, 1998c), and C_2H_2 (Zheng & Srivastava 1996). Theoretical ionization cross sections are available for H_2, N_2, O_2, CO, H_2O, and CO_2 (Hwang et al. 1996), H_2O (Liu et al. 1997), and C_{60} (Deutsch et al. 1996) and Majeed & Strickland (1998) have compiled ionization data for N_2 and O_2. A recommended H_2 dissociation cross section has been constructed by Martin et al. (1998).

The process of dissociative recombination (DR) in which an electron is captured by a molecular ion with the resulting neutral intermediary dissociating into a number of neutral products is an important process in many astrophysical environments. DR is an efficient mechanism for producing complex neutral molecules, but it has proven difficult to study experimentally and theoretically. However, the recent development of heavy-ion storage rings has allowed for accurate determinations of low-energy cross sections and product-state branching ratios, the latter of great importance to astrochemical studies of interstellar clouds. An improved understanding of the reaction mechanism has also allowed for accurate calculations with multichannel quantum defect and R-matrix methods. Molecular ions which have been studied during the report period include H_2^+ (van der Zande et al. 1996), HeH^+ (Orel & Kulander 1996; Strömholm et al. 1996), H_2O^+ and H_3O^+ (Vejby-Christensen et al. 1997), CH_2^+ (Larson et al. 1998), CH_3^+ (Vejby-Christensen et al. 1997), CH_5^+ (Semaniak et al. 1998), CN^+ (Le Padellec et al. 1999), CO^+ (Rósen et al. 1998), and HCO^+ (Le Padellec et al. 1997).

Recent work on elastic collisions between electrons and molecules include H_2 and N_2 (Isaacs & Morrison 1996), NO (Da Paixao et al. 1996), CO_2 (Gianturco & Stoecklin 1996), CO (Gibson et al. 1996), CO_2 (Takekawa & Itikawa 1996), O_2 (Green et al. 1997), H_2O (Gianturco et al. 1998a), O_3 (Sarpal et al. 1998), CO_2 (Tanaka et al. 1998), CO, N_2, NO, and O_2 (Liu & Sun 1996), and CO, CO_2, CH_4, C_2H_4, and C_2H_6 (Maji et al. 1998).

3.3. Ion-Atom and Atom-Atom Collisions

Though a very large range of species involved in ion-atom and atom-atom collisions has recently been studied, of principal interest in astrophysics have been collisions involving the abundant species such as H, H_2, He, C, N, and O.

For example, chemistry in nebulae often involves the transfer of an electron between ions and atoms through low energy collisions, or strong magnetic fields can accelerate ions which precipitate into the atmospheres of planets or stream through clouds of ejecta, capturing electrons from the gas atoms. Recent works have considered charge transfer in the following collisions: O^{3+} + H (Beijers et al. 1996), H^+ + C, N, O, Si (Kimura et al. 1997), C^+ + H (Stancil et al. 1998a), N^{2+} + H (Pieksma et al. 1997), Si^{4+} + H, D (Wu & Havener 1997), C^{5+} + He (Fritsch & Lin 1996), Si^{3+} + He (Fang & Kwong 1997; Stancil et al. 1999), O^+ + O (Hickman et al. 1997), and C^{2+} + He (McCullough et al. 1997). Kingdon & Ferland (1996) have provided analytical fits for low-energy charge transfer between multiply-charged ions and H and made them available on the WWW. Cross sections have been computed for charge transfer between H and all H-like ions by Harel et al. (1998) and for resonant charge transfer of neutral and singly ionized atoms from H to Ca (Copeland & Crothers 1997).

Of particular importance to transport in H/H_2 plasmas, such as planetary ionospheres, the heliospheric shock interface with the ISM, comet bow shocks, *etc.*, is the elastic scattering cross section and its related moments (e.g. momentum transfer and viscosity cross sections). Recent work has computed the elastic differential cross section at a large number of energies between 0.1 and 100 eV and the corresponding integral elastic and transport moments for H^+, D^+, H, D + H, D, He (Krstić & Schultz, 1999) and provided a WWW interface to the raw data. This work also cites a large part of the relevant extant literature regarding elastic collisions involving H, H_2, and He.

For thermal (e.g., ∼100-10,000 K) plasmas or for ions accelerated by strong fields (e.g. 10^4-10^7 K) excitation and ionization can also be of significant interest. Notable examples of results for excitation include proton impact excitation for Be-like (Ryan et al. 1998), B-like (Foster et al. 1997), C-like (Ryan et al. 1999), and Be-like to Cl-like ions (Copeland et al. 1997). Regarding ionization, the following works are of particular interest: He^* + H (Mihajlov et al. 1996), H + H (Krstić et al. 1996), H^+ + O (Thompson et al. 1997), H^+, He^{2+}, Li^{3+} + H (Toshima 1997), and H^+ + H (Shah et al. 1998).

Ion-atom and atom-atom collisions can also create molecules through radiative association and associative attachment. Babb & Kirby (1998) have surveyed the available literature up to 1997. More recent results include radiative association formation of HeH^+ (Zygelman et al. 1998), CO, CS^+, and SiN (Singh et al. 1999), C_2, C_2^+, N_2^+, and Si_2 (Andreazza & Singh 1997).

Also noteworthy is the fact that an increasing number of investigations are seeking to provide information about atomic collisions involving strong external fields, and may soon provide new data needed in astrophysical modeling. Furthermore, a number of recent works have shown that the generally expected smooth decline of inelastic (e.g. excitation, ionization, non-resonant charge transfer) cross sections toward threshold, down from their peak at higher energies, might quite ubiquitously have oscillations superimposed (Schultz et al. 1997; Horvath et al. 1996; Krstić et al. 1998; DeHeer et al. 1992).

3.4. Ion-Molecule and Atom-Molecule Collisions

For astrophysical gas at lower temperatures and higher densities, collisions of ions and atoms with molecules become increasingly important. Examples include the precipitation of accelerated ions into a dense planetary atmosphere and dense primordial clouds cooled by radiating molecules excited through collisions.

Regarding charge transfer for ion-molecule collisions, recent works of interest include the following collisions: N^+ + H_2O (Dressler et al. 1995), O^{3+} + H_2 (Beijers et al. 1996), C^{2-4+} + H_2, CH_4, CO_2 (Itoh et al. 1995), H^+, D^+ + H_2 (Ichihara et al. 1996), He^{2+}, Li^{3+}, C^{4+}, N^{5+} + H_2 (Kumar & Saha 1998), H^+ + C_2H_2 (Kimura et al. 1996), C^{2+} + H_2 (McCullough et al. 1997), H^+ + N_2, O_2 (Siegmann et al. 1998), and O^+ + N_2 (Lindsay et al. 1998).

As described above, a recent work has extensively investigated the elastic and transport cross sections for H/H_2 plasmas/gases and provides on the WWW tabulations of the differential and integral cross sections for H^+, D^+, H, D + H_2, D_2, HD (Krstić & Schultz 1999).

Rotational and vibrational excitation of molecules is the primary mechanism for populating excited rovibrational states and for radiative cooling in low ionization environments. Rate coefficients have been computed for rovibrational excitation of H_2 by H, He, and H_2 impact (Le Bourlot et al. 1999; Balakrishnan et al. 1997, 1999; Forrey et al. 1997); of HD by H (Roueff & Flower 1999), He (Roueff & Zeippen 1999), and H_2 impact (Flower 1999); and of CO by H impact (Green et al. 1996). Also of interest are recent works describing ionization of astrophysically important molecules: He^* + H_2O, H_2, N_2 by Ishida (1996), Vojtik (1996), and Ishida & Horime 1996), respectively, H + N_2 (Quintana & Pollack 1996), and He^+ + H_2 (Hsu et al. 1996),

Of significant interest to circumstellar, interstellar, primordial cloud, planetary atmosphere and other environments, in which molecules can survive, is dissociation. Recent works of interest include the following: H, He, H_2 + H_2 (Martin et al. 1998), He + H_2 (Sakimoto 1997), He + HeH^+ (Coelho et al. 1996; Prior & Brauning 1998), H^+, He^+, O^{6+} + H_2O, N_2 (Werner et al. 1997), He + H_3^+ (Peko et al. 1996), He + CO_2^+ (Bhardwaj et al. 1998), He^{2+} + CO (Folkerts et al. 1997), H^+, Li^{2+}, C^{3-6+}, F^{4-9+}, $Si^{9-11,17+}$ + H_2, CO, CH_4 (Ben-Itzhak et al. 1997), Na^{2+} + H_2 (Fayeton et al. 1998), and He^* + CO_2 (Arfa et al. 1998). Of course, the formation of molecules precedes their dissociation (cf. review by Babb & Kirby 1998 on association processes). A recent study of the formation of CH_5^+ by the radiative association of CH_3^+ with H_2 was given by Talbi & Bacchus-Montabonel (1998).

3.5. Reactive Scattering and Chemistry

There is insufficient space to review the advances in reactive scattering. Therefore, we refer the reader to the following compilations. A database of 3864 gas-phase reactions important for interstellar and circumstellar chemistry has been compiled by Millar, Farquhar, & Willacy (1997). The reaction rate coefficient fits are available on the WWW. Stancil, Lepp, & Dalgarno (1996, 1998b) and Abel et al. (1997) have compiled a set of gas-phase reaction rate coefficients for primordial gas (H, D, He, and Li) with the latter available on the WWW. Two important experimental studies are worth mentioning: Canosa et al.

(1997) have studied reactions of CH with a number of complex hydrocarbons and Decker, Adams, & Babcock (1999) have investigated HS_2H^+ colliding with a variety of complex molecules.

Acknowledgments. The work of D. R. S. was supported by the U. S. Department of Energy under Contract DE-AC05-96OR22464 and that of P. C. S. by a grant from the NASA AISR Program.

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