

Commission 14: Atomic & Molecular Data

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Abstract. This triennial report from Comm. 14 covers the topics Atomic Spectra and Wavelength Standards, Atomic Transition Probabilities, Collision Processes, and Line Broadening.

Commission 14 belongs to Division XII of the IAU. The rôle of Commission 14 is to inform the astronomical community of new developments in the diverse fields of research and measurement that involve atoms, molecules and solid state particles. Conversely, it endeavors to sensitize the research communities active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commission 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 astronomical community. It comprises Sections prepared by four of the eight Working Groups of Commission 14. It is also available on the Commission 14 web site.

1. WORKING GROUP ON ATOMIC SPECTRA AND WAVELENGTH STANDARDS

CHAIR: S. Johansson
CO-CHAIR: G. Nave

1.1. *Energy Level Analyses, Wavelengths and Line Classifications*

The references cited in this section are mostly papers on original laboratory research; compilations and data bases are covered in another section. The references, ordered by atomic number and spectrum, are given in parentheses following the spectral notations. They are designated by the first letter of the first author's last name and a serial number; these designations precede the full citations in the reference list at the end of the report.

H I, **D I** (K1), **H I** (K6) hfs, **Li I** (D2), **Li I** (W1) hfs, **B II** (M1,R1), **Ne I** (S4), **Ne III** (K5), **Ca I** (M4) hfs, **Sc I** (B2) hfs, **Ti I** (L3), **Ti IV** (R2), **V I** (L1) hfs, **Mn I** (B1, L2) hfs, **Mn II** (B5) hfs, **Cr II** (S5), **Ni VII** (K7), **Sr II** (B3) hfs, **Y I** (N2) hfs, **Nb I** (B4) hfs, **Mo II** (N1), **Cs II** (S6), **Sm I** (O1) hfs, **Sm II** (M5) hfs, **Bi II** (D3), **Pt I,II** (N3, S5), **Ta I** (M2), **Ta I** (J1) hfs, **Ta II** (E1,M3,Z1) hfs, **Ta III** (A1).

The references for elements heavier than Ni ($Z > 28$) are limited to the first three or four spectra only, these data being of interest for solar and stellar spectroscopy. The references of the lighter elements are also incomplete, the selection being limited to those

of highest astrophysical interest. The quality of astrophysical spectra sometimes requires that hyperfine structure (hfs) is considered in the analysis. We have therefore included some experimental data on hfs.

Current work in term analyses of high-resolution laboratory spectra (energy levels, wavelengths) of the lowest ionization stages of astrophysical significance is ongoing at Lund, Sweden (transition elements and rare earth elements), London, UK (iron group elements), NIST, USA (heavy elements, rare earths), Troitsk, Russia (heavy elements), Antigonish, Canada (higher ionization states, heavy elements) and Meudon & Orsay, France (transition groups, theory). A number of laboratories are involved in measurements of hfs.

1.2. Wavelength Standards

Based on the refined energy levels of **H & D** (K1) accurate wavelengths have been derived for these H isotopes (see Reader, 2004). Banerjee, Das, & Natarajan (2004) present frequency measurements with an accuracy of 0.7 mÅ of the resonance lines of **K I**, which can be used to test calibration lines. Nave & Sansonetti (2004) give reference wavelengths of **Fe I**, **Ge I** & **Pt I** lines in a region around 1935 Å. A similar work on **U I** & **Th I** in a limited wavelength region (6040-7550 Å) is published by Degraffenreid & Sansonetti (2002, D1). Accurate wavelengths for ground state lines in **Ti II**, **Cr II**, **Mn II**, **Fe II** & **Ni II** have been measured in a single spectrum from a composite hollow-cathode lamp (Aldenius, Johansson & Murphy 2005). Fourier Transform Spectrometry has been used at NIST to measure calibration wavelengths of mono-isotopic mercury, ¹⁹⁸Hg (Salit *et al.* 2004; Veza *et al.* 2005)

1.3. Larger Compilations, Reviews, Conference Proceedings

A number of compilations on wavelengths and energy levels have been published or submitted by the spectroscopy group at NIST:

Be II (K3), **Ne I** (S2), **Ga I-XXXI** (S9), **KrI-XXXVI** (S3), **RbI-XXXVII** (S8), **XeI-LIV** (S1), **BaI-II** (C1), **WII-II** (K4), and special compilations of X-ray data for the Chandra Observatory: **NeV-VIII** (P4), **MgV-X** (P3), **SiVI-XII** (P2), **S VII-XIV** (P1). Ionization energies for tungsten (W^{2+} to W^{71+}) are compiled by Kramida & Reader (2005). Morton (2003) has continued with a third compilation on *Atomic Data for Resonance Absorption Lines*, which concerns wavelengths longward of the Lyman Limit for H-Ga.

A number of papers on atomic spectroscopic data are included in proceedings of the *Eighth International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, held in Madison, WI, USA, August 2004. Invited papers are published in the Physica Scripta T Series (Lawler, Wahlgren & Wiese 2005). A few papers on astrophysical data needs are included in the proceedings from the third and fourth international conferences, *ICAMDATA*, held at Gatlinburg, Tn, USA, in April 2002 (Shultz, Krstic & Ownby 2002), and at Toki, Japan in October 2004 (Kato, Kato & Funaba 2005), respectively. The proceedings contain review papers as well as descriptions of atomic and molecular databases. Proceedings from the EGAS (European group of Atomic Spectroscopy) conferences appear in the Physica Scripta T-series: 31st EGAS T86 (2000) and 32nd EGAS T95 (2001).

1.4. Atomic Spectroscopic Data on the Internet

A comprehensive bibliographic database on atomic spectroscopy with a search engine on various atomic parameters is available at the Institute of Spectroscopy, Troitsk, at the URL address: <http://das101.isan.troitsk.ru/bibl.htm>.

The database DREAM is devoted to the rare-earth elements in the low ionization stages. It contains presently data for over 60 000 transitions, many of them of astrophysical interest. More details can be found on the Web site: <http://www.umh.ac.be/astro/dream/shtml>. The database has been described recently in Biémont & Quinet (2005). A set of databases (R4) are available at NIST at following URL addresses:

<http://physics.nist.gov/Handbook>

This handbook by Sansonetti & Martin (S7) includes about 10000 wavelengths for the strongest lines of all elements H-Es for neutral and singly-ionized atoms, with ionization energies, transition probabilities, line classifications, isotope information and references.

URL:<http://physics.nist.gov/ASD>

The Atomic Spectra Database (R3) version 3.0 is fully revised since last report with new Web interface. Many new data, corrected errors, online generation of Grotrian diagrams, Saha/LTE spectra and direct access to references. Versions 2.0 and 1.3 are archived and will not be updated.

<http://physics.nist.gov/Chandra>.

This X-ray database for the Chandra Observatory (P5) contains Wavelengths, energy levels and transition probabilities for lines between 20 Å and 170 Å for Ne, Mg, Si and S ions

<http://physics.nist.gov/IonEnergy>

The database (M6) gives Ground Levels and Ionization Energies for the Neutral Atoms of 9 elements.

<http://physics.nist.gov/HDEL>

Theoretical values of energy levels of H and D for quantum numbers $n = 1$ to 200.

An Atomic Energy Levels and Spectra Bibliographic Database is in preparation. It contains about 8500 references between July 1968–December 2000 on atomic energy levels and spectra. It will be merged with the transition probability and line broadening bibliographic databases.

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2. WORKING GROUP ON ATOMIC TRANSITION PROBABILITIES

CHAIR: G. M. Wahlgren

CO-CHAIR: J. R. Fuhr

Members of the astronomy and physics communities continue to produce new data on transition probabilities and oscillator strengths that are crucial to spectral analysis of astronomical objects. The techniques include laboratory experiment, *ab initio* calculations and direct inference from stellar spectra. In addition to creating new data, progress continues in providing easily accessible data sets.

The attached bibliography for the period 2002–2005 consists of 182 references. Of these, 145 publications involve quantum mechanical calculations, many as the sole technique. The reference list of ions is represented by 96 elements and a wide range of ionic states. The distribution among ions states is not equitable, but reflects two groupings: the lowest three ions and the highest ionization states.

The distribution by spectrum also reflects the techniques employed. Studies of high-ionization states are invariably of a theoretical nature, while those for the lowest ionization states include all of the experimental analyses reported. Among the experimental works, the techniques involve study of emission lines and the recording of atomic lifetimes, usually by the method of laser-induced fluorescence. The maturity of this technique is now providing benefits to many applications. The application of absorption spectroscopy appears currently to be a rare occurrence.

It is also apparent that work on atomic data is generally motivated by the needs of astronomical-based projects, and not to enhance the overall knowledge of atomic parameters. Of continued interest have been elements from the iron group, the lanthanides, and even heavier stable elements. The experimental work conducted in support of these programs is limited to the neutral and two lowest ions by available instrumentation and light sources, often being hollow-cathode designs.

The following major compilations of transition probability data have been published during the latest 3-year period:

(a) The MCHF/MCDHF Collection on the Web has been established by C. Froese Fischer *et al.*: http://www.vuse.vanderbilt.edu/~cff/mchf_collection/. It contains a large number of transitions for Li-like through Ar-like ions of various chemical elements,

principally the lighter elements through atomic number $Z = 30$. The data include various types of electric-dipole forbidden lines and are obtained from sophisticated multi-configuration Hartree Fock (MCHF) or, for the heavier, more highly ionized species, from multi-configuration Dirac Hartree Fock (MCDHF) calculations. The tabulations provide data for fine-structure transitions and include other important spectroscopic data for each line, and are structured similar to the NIST tables. Another large compilation was recently published: Breit-Pauli energy levels, lifetimes, and transition probabilities for the beryllium-like to neon-like sequences, C. F. Fischer and G. Tachiev, *At. Data Nucl. Data Tables* 87, 1–184 (2004).

(b) Transition probabilities for the resonance lines of selected elements have been compiled by Morton: Atomic data for resonance absorption lines. III. Wavelengths longward of the Lyman limit for the elements hydrogen to gallium, D. C. Morton, *Astrophys. J., Suppl. Ser.* 149, 205–238 (2003); Erratum: 151, 403 (2004).

(c) NIST Atomic Transition Probabilities, J. R. Fuhr and W. L. Wiese, in *CRC Handbook of Chemistry and Physics*, 86th Edition, 10-93-10-155 (Edited by D. R. Lide, CRC Press, Boca Raton, FL, 2005)

The use of electronic databases continues to grow as more data and bibliographies are made available in this medium. Several of the most useful databases active during this reporting period include:

(a) Version 7.0 of the NIST Atomic Transition Probability Bibliographic Database now contains 6570 references, dating from 1914 through June 2002. For this version, 454 bibliographic entries have been added.

(b) The availability of transition probability and oscillator strength data computed under the TOPbase and Opacity Projects is accessible at <http://vizier.u-strasbg.fr/topbase/topbase.html> for astrophysically abundant ions ($Z \leq 26$). The OPserver at this site allows opacity calculations for arbitrary chemical mixtures.

(c) The D.R.E.A.M. database (Database on Rare Earths at Mons University) continued to have data added for wavelengths, energy levels, oscillator strengths and radiative lifetimes for neutral, singly and doubly-ionized rare earth elements. These data reflect input from calculations, lifetime measurements, and experimental branching fractions.

Discussions around the availability of data, along with the presentation of techniques, continued through the proceedings of the 8th International Colloquium on Atomic Spectra and Oscillator Strengths (ASOS8) [105]. Several review articles present techniques in determining experimental oscillator strengths, including the laser-induced fluorescence, electron-beam ion-traps, and storage rings.

The main body of this report is a bibliography of selected recent literature references, which contain new transition probability data of astrophysical interest produced during the last three-year period. Thus, this new selected bibliography continues where the last working group left off. As in the previous reports, the bibliographical material is ordered with respect to element and stage of ionization. One table provides an overview of the bibliographical data by spectrum. We were selective in our choice of these references, i.e., all papers had to contain a significant amount of numerical data, normally for more than

ten spectral lines. The references are identified by a running number, which refers to the general reference list given in this report. In the general reference list, the literature is ordered alphabetically according to the first author, and each reference contains one or more code letters indicating the method applied by the authors. These code letters are defined as follows:

THEORETICAL METHODS:

~ Q quantum mechanical calculations

EXPERIMENTAL METHODS:

~ A measurements in absorption (absorption tube, etc.)

~ E measurements in emission (arc, hollow cathode, etc.)

~ L lifetime measurements (laser-induced fluorescence, beam-laser and beam-foil spectroscopy, etc.)

~ M miscellaneous experimental methods (for example, Stark effect, astrophysical measurements, etc.)

OTHER:

~ CP data compilations

~ CM comments

~ F forbidden transitions (not electric dipole)

~ R relative values only

Table 1. Important Literature References

Ac LXXVII: 139	Ar XV: 115, 121	Bi LXXI: 139
Ac LXXXII: 174	Ar XVI: 112, 115, 121	Bi LXXVI: 174
	Ar XVII: 115, 121, 140	
Ag XXXV: 139		Bk LXXXV: 139
Ag XL: 174	As XXI: 139	
	As XXVI: 174	Br XXIII: 139
Al I: 18		Br XXVIII: 174
Al II: 177	At LXXIII: 139	
Al VI: 99	At LXXVIII: 174	C I: 44, 73, 167, 168, 176
		C II: 50
Am LXXXIII: 139	Au LXVII: 139	C III: 74
	Au LXXII: 174	C IV: 6
Ar I: 14, 85		C V: 140
Ar V: 157	B II: 74	
Ar VI: 77, 139		Ca I: 18, 44, 68
Ar VII: 67	Ba I: 52	Ca VII: 102
Ar XI: 99, 115, 121, 174	Ba II: 52	Ca VIII: 101, 139
Ar XII: 66, 115, 121	Ba XLIV: 139	Ca IX: 94, 150
Ar XIII: 1, 106, 115, 121	Ba XLIX: 174	Ca XIII: 99, 174
Ar XIV: 1, 115, 121		Ca XIX: 95

Table 1. Important Literature References (cont.)

Cd I: 160	Cu XVII: 139	Ga XIX: 139
Cd II: 111, 160	Cu XXII: 99, 174	Ga XXIV: 174
Cd XXXVI: 139		
Cd XLI: 174	Dy III: 175	Gd I: 159
	Dy LIV: 139	Gd II: 159
Ce I: 163	Dy LIX: 174	Gd III: 34
Ce II: 163		Gd LII: 139
Ce III: 35	Er I: 164	Gd LVII: 174
Ce XLVI: 139	Er II: 158	
Ce LI: 174	Er LVI: 139	Ge XX: 139
	Er LXI: 174	Ge XXV: 174
Cf LXXXVI: 139		
	Es LXXXVII: 139	Hf LX: 139
Cl I: 19		Hf LXV: 174
Cl II: 19, 58, 141, 147, 149	Eu III: 133	
Cl III: 19, 141	Eu LI: 139	Hg LXVIII: 139
Cl IV: 19	Eu LVI: 174	Hg LXXIII: 174
Cl V: 19, 47, 139		
Cl VI: 19, 67, 123	Fe I: 44	Ho I: 122
Cl VII: 19	Fe II: 13, 49, 82, 89, 126, 128, 138, 142	Ho II: 104
Cl VIII: 19	Fe III: 126	Ho LV: 139
Cl IX: 19	Fe IV: 70, 118, 126	Ho LX: 174
Cl X: 19, 41, 99, 174	Fe V: 126	
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Cl XII: 19	Fe VII: 126, 170	I XLVI: 174
Cl XIII: 19	Fe VIII: 126, 171, 172	
Cl XIV: 19	Fe IX: 126, 171	In II: 125
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Cm LXXXIV: 139	Fe XIII: 4, 153, 156, 157, 166	Ir I: 87
	Fe XIV: 15, 75, 139	Ir II: 86
Co XV: 139	Fe XV: 96	Ir LXV: 139
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Cr II: 18	Fe XX: 90, 119, 127	K VIII: 37, 56
Cr VIII: 114	Fe XXI: 127	K XII: 99, 174
Cr XII: 139	Fe XXII: 127	K XIV: 7
Cr XVII: 99, 174	Fe XXIII: 127	
Cr XIX: 7	Fe XXIV: 71, 112, 127	Kr I: 14
	Fe XXV: 127	Kr XXIII: 157
Cs XLIII: 139		Kr XXIV: 139
Cs XLVIII: 174	Fm LXXXVIII: 139	Kr XXIX: 174
Cu II: 65	Fr LXXV: 139	La I: 31
Cu XIV: 152	Fr LXXX: 174	La II: 62, 138

Table 1. Important Literature References (cont.)

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La L: 174	Ne VI: 129	
	Ne VII: 129, 173	Po LXXII: 139
Lu I: 53	Ne VIII: 129	Po LXXVII: 174
Lu LIX: 139	Ne IX: 140	
Lu LXIV: 174		Pr I: 30
	Ni I: 18, 88	Pr II: 33, 144
Mg I: 18	Ni IV: 113	Pr XLVII: 139
Mg II: 46, 108, 109	Ni XII: 145	Pr LII: 174
Mg V: 99, 130	Ni XIII: 10, 152	
Mg VI: 130	Ni XIV: 10	Pt I: 60
Mg VII: 130	Ni XV: 10	Pt LXVI: 139
Mg VIII: 130	Ni XVI: 10, 75, 139	Pt LXXI: 174
Mg IX: 130	Ni XVII: 57	
Mg X: 130	Ni XVIII: 134, 137	Pu LXXXII: 139
Mg XI: 165	Ni XXI: 26, 99, 174	
	Ni XXV: 154	Ra LXXVI: 139
Mn I: 39		Ra LXXXI: 174
Mn II: 151	Np LXXXI: 139	
Mn XIII: 139		Rb XXV: 139
Mn XVIII: 99, 174	O I: 73, 176, 180	Rb XXX: 174
Mn XX: 7	O II: 180	
	O III: 180	Re LXIII: 139
Mo II: 124	O IV: 50, 97, 116, 169, 180	Re LXVIII: 174
Mo XXX: 139	O V: 16, 117, 180	
Mo XXXV: 174	O VI: 5, 180	Rh XXXIII: 139
	O VII: 140	Rh XXXVIII: 174
N I: 179		
N III: 50, 64	Os I: 87	Rn I: 14
N IV: 16, 64	Os II: 86	Rn LXXIV: 139
N V: 64	Os LXIV: 139	Rn LXXIX: 174
N VI: 140	Os LXIX: 174	
		Ru XXXII: 139
Na I: 146	P II: 148	Ru XXXVII: 174
Na III: 83	P III: 78, 139	
Na IV: 99	P IV: 67, 79	S II: 84
	P VIII: 99, 174	S IV: 139
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Si III: 63	Te XL: 139	Xe XLII: 139
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3. WORKING GROUP ON Collision Processes

PRESIDENT: D.R. Schultz and P.C. Stancil

Since the last working group report in 2002, very active research continues that spans the vast range of atomic and molecular collision processes of interest in astrophysics. Given the large volume and scope of the pertinent published literature and the limited space available here, rather than seeking to comprehensively review this progress, we have attempted to identify works and some compilations of particular importance. In addition, access to an on-line bibliographic database that can be searched by collision reaction category, reactants, authors, and dates is made available by the Oak Ridge National Laboratory Controlled Fusion Atomic Data Center (CFADC 2005). Since a very high level of overlap exists between the atomic and molecular data needs of plasma science relevant to fusion energy and to astrophysics, this database, containing entries from 1978 to present, should be quite useful for those seeking such information. In addition, categorized bibliographies based largely on the bibliographic data compilation of the ORNL CFADC have been published in hardcopy by the International Atomic Energy Agency (CIAMDA 1998).

Here we organize our report summarizing new work on relevant collision processes including electron impact on atoms, ions, molecules, and molecular ions; ion-atom and atom-atom collisions; ion-, atom-, and molecule-molecule collisions; and reactive scattering and chemistry.

3.1. *Electron Collisions with Atoms, Ions, Molecules, and Molecular Ions*

Collisions of electrons with atoms, ions, molecules, and molecular ions are the major excitation mechanism in a wide range of astrophysical environments. In addition, they largely drive ionization and recombination, contribute to molecular fragmentation and formation, and influence transport. In the following sections we summarize recent work of interest for electron collisions with astrophysically relevant species regarding elastic scattering, excitation, dissociation, ionization, recombination, and electron detachment from negative ion since the time of the last Commission report (Schultz & Stancil 2002).

3.2. *Electron-Atom Scattering*

New references for elastic scattering from atoms are as follows: H (Papp & Hu 2002, James, Childers & Khakoo 2004, Witthoef, Loch & Pindzola 2004, Jablonski, Salvat & Powell 2004), noble gases (Garcia *et al.* 2002—Ne, Ar, Kr, Xe; Baek & Grosswendt 2003—He, Ne, Ar; Demesie *et al.* 2003—Xe; Blanco & Garcia 2003—He, Ne, Ar, Kr, Xe; Date, Ishimaru & Shimozuma 2003—Xe; Salvat 2003—He, Ne, Ar, Kr, Xe; McEachran & Stauffer 2003—Kr; Ariyasinghe & Goains 2004—Kr, Xe; Cho *et al.* 2004b—Kr; Milosavljevic, Sevic & Marinkovic 2004—Kr), O (Plummer, Noble & Le Dourneuf 2004), Mg (Al-Mulla & Joensson 2002, Bartschat & Sadeghpour 2003, Bartschat *et al.* 2004), Al (Jablonski, Salvat & Powell 2004), Ca (Bartschat & Sadeghpour 2003), Ni (Jablonski, Salvat & Powell 2004), and Zn (Sienkiewicz *et al.* 2002).

Excitation of atoms are covered in new references: H (Sweeney *et al.* 2001, Kim 2001, James *et al.* 2002, Sweeney, Grafe & Shyn 2004, James, Childers. & Khakoo 2004, Witthoef, Loch. & Pindzola 2004), He (Kim 2001, Dogan & Crowe 2002, Mityureva, Smirnov & Ponomarenko 2002, Bartschat & Andersen 2003, Baek & Grosswendt 2003, Harries, Hammond & Murray 2003, Merabet *et al.* 2003b, Kheifets 2004), Li (Kim 2001, Griffin *et al.* 2001, Witthoef *et al.* 2003), Be (Kim 2001, Ballance *et al.* 2003b), C (Srivastava, McEachran & Stauffer 2002, Kim & Desclaux 2002, Zatsarinny & Fischer 2002), N (Kim & Desclaux 2002), O (Zatsarinny & Tayal 2002a, Kim & Desclaux 2002, Tayal 2002, Johnson *et al.* 2003a, Johnson *et al.* 2003b, Plummer, Noble & Le Dourneuf 2004), Ne (Boffard *et al.* 2001, Khakoo *et al.* 2002, Stewart *et al.* 2002, Meneses *et al.* 2002, Baek & Grosswendt 2003, Zatsarinny & Bartschat 2004a, Ballance & Griffin 2004), Mg (Fursa & Bray 2001, Kim 2001, Kai *et al.* 2004), Si (Srivastava, McEachran. & Stauffer 2002), S (Zatsarinny & Tayal 2002b), Ar (Stewart *et al.* 2002, Baek & Grosswendt 2003, Weber, Boffard & Lin 2003, Madison *et al.* 2004, Zatsarinny & Bartschat 2004b), Ca (Kim 2001, Muktvat, Srivastava & Stauffer 2002), Kr (Stewart *et al.* 2002, Yuan *et al.* 2002, Tsurubuchi Kobayashi & Hyodo 2003, Li *et al.* 2003, Yu *et al.* 2003, Cho *et al.* 2004b), and Xe (Kanik, Johnson & James 2001, Boechat-Roberty *et al.* 2002, Yu *et al.* 2003, Date, Ishimaru & Shimozuma 2003, Bartschat, Dasgupta & Madison 2004).

New publications on ionization include: H (Deb & Crothers 2002, Lepp, Stancil & Dalgarno 2002, Isaacs *et al.* 2001, Szluniska, Van Reeth & Laricchia 2002, Bartlett, Stelbovics & Bray 2003, Childers *et al.* 2003, Bartlett & Stelbovics 2004, Chen *et al.* 2004, Childers *et al.* 2004), He (Lepp, Stancil & Dalgarno 2002, Dogan & Crowe 2002, Denifl *et al.* 2002, Keller 2003, Bray, Fursa & Stelbovics 2003, Fursa & Bray 2003, Merabet *et al.* 2003a, Defrance, Kereselidze & Machavariani 2003, Merabet *et al.* 2003b, Kheifets & Bray 2004, Sorokin *et al.* 2004, Kheifets 2004, Pindzola *et al.* 2004, Uddin *et al.* 2004b), noble gases (Rejoub, Lindsay & Stebbings 2002 - He, Ne, Ar, Kr, Xe; Kobayashi *et al.* 2002 - Ne, Ar, Kr, Xe; Bartlett & Stelbovics 2002 - Ne, Ar, Kr, Xe; Gstir *et al.* 2002 - Ne, Ar, Xe; Szluniska, Van Reeth & Laricchia 2002 - He, Ne, Ar, Kr, Xe; Gstir *et al.* 2003 - He, Ne, Ar, Kr, Xe; Erwin & Kunc 2003 - Ar, Kr, Xe, Rn), Li (Huang *et al.* 2002, Ghosh & Sinha 2003), C (Kim & Desclaux 2002, Szluniska, Van Reeth & Laricchia 2002, Alfaz Uddin & Basak 2003a), N (Kim & Desclaux 2002, Szluniska, Van Reeth & Laricchia 2002, Alfaz Uddin & Basak 2003a), O (Kim & Desclaux 2002, Szluniska, Van Reeth & Laricchia 2002, Joshipura, Antony & Vinodkumar 2002, Alfaz Uddin & Basak 2003a), Mg (Kampp *et al.* 2002, Jha & Roy 2002), Si (Bartlett & Stelbovics 2002), P (Bartlett & Stelbovics 2002), S (Bartlett & Stelbovics 2002), Ar (Biava *et al.* 2002, Stano *et al.* 2003, Cooper & van Boeyen 2004), Ca (Alfaz Uddin & Basak 2003b), Ti (Alfaz Uddin & Basak 2003b), Cr (Alfaz Uddin & Basak 2003a), Mn (Llovet, Merlet & Salvat 2002, Alfaz Uddin & Basak 2003a), Fe (Llovet, Merlet & Salvat 2002, Alfaz Uddin & Basak 2003a), Kr (Denifl *et al.* 2002, Loch *et al.* 2002), Xe (Date, Ishimaru & Shimozuma 2003), and series of atoms (Santos, Parente & Kim 2003 - C, N, O, Ne, Mg, Al, Si, P, S, Ar, Ti, Cr, Fe, Co, Ni, Kr).

Negative ion formation (i.e. $e + A \rightarrow A^-$) has been studied for: H (Ghosh, Nath & Sinha 2003, Grujic 2003, Fritioff *et al.* 2004), Li (Le Padellec *et al.* 2002), and S (Fritioff *et al.* 2003).

3.3. Electron-Ion Scattering

New elastic data exists for He^+ (Bhatia 2002).

New work for excitation of atomic ions include: He^+ (Kim 2002, Witthoef, Pindzola & Colgan 2003), He-like (Whiteford *et al.* 2001 - Ar, Fe; Zhang & Sampson 2002 - O,

Fe), Li⁺ (Ballance *et al.* 2003a), Li-like (Whiteford *et al.* 2002 - Ar, Fe; Starobinets *et al.* 2003 - Be, B), Be-isonuclear (Ballance *et al.* 2003b - Be^{+−3+}), C²⁺ (Mitnik *et al.* 2003), C³⁺ (Aggarwal & Keenan 2004a), O²⁺ (Niimura, Smith & Chutjian 2002), O³⁺ (Smith *et al.* 2003), O⁶⁺ (Delahaye & Pradhan 2002), O⁷⁺ (Berrington & Ballance 2002), Ne²⁺ (McLaughlin, Daw & Bell 2002), Ne⁸⁺ (Bautista 2003), Ne-like (Brown, Beiersdorfer & Widmann 2001 - Fe, Co, Ni, Kr), Mg⁺ (Kim 2002), Mg-like (Kai, Srivastava & Nakazaki 2004 - S, Ar, Ca), Al²⁺ (Dunn *et al.* 2002, Bannister *et al.* 2002, Smith *et al.* 2003), Si⁶⁺ (Bhatia & Landi 2003), Si²⁺ (Janzen *et al.* 2003, Smith *et al.* 2003), P²⁺ (Gupta & Msezane 2002), Ar⁶⁺ (Smith *et al.* 2003), Ar⁷⁺ (Smith *et al.* 2003), Ca⁶⁺ (Landi & Bhatia 2003), Ca⁷⁺ (Landi, Storey & Zeippen 2004), Ca¹⁴⁺ (Aggarwal & Keenan 2002, Aggarwal & Keenan 2003b), Ti²⁺ (Popovic *et al.* 2002), Fe⁺ (Burke *et al.* 2002, Ramsbottom *et al.* 2002, Ramsbottom *et al.* 2004), Fe²⁺ (McLaughlin *et al.* 2002), Fe⁴⁺ (Woeste *et al.* 2002), Fe⁸⁺ (Storey, Zeippen & Le Dourneuf 2002), Fe¹⁰⁺ (Aggarwal & Keenan 2003a), Fe¹²⁺ (Aggarwal & Keenan 2004b, Aggarwal & Keenan 2005), Fe¹⁴⁺ (Aggarwal, Keenan & Msezane 2003), Fe¹⁶⁺ (Chen, Pradhan & Eissner 2003), Fe²¹⁺ (Gu 2004), Fe²³⁺ (Pindzola 2002, Bautista *et al.* 2003), Fe²⁵⁺ (Ballance, Badnell & Berrington 2002), Fe-isonuclear (Bautista *et al.* 2004 - Fe^{16−22+}), Ni⁺ (Bautista 2004), Ni⁴⁺ (Burke *et al.* 2002), Ni²⁴⁺ (Chidichimo, Badnell & Tully 2003), Zn⁺ (Kim 2002), and Xe²⁶⁺ (Badnell *et al.* 2004).

Ionization and detachment have been studied for: H[−] (Ghosh, Nath & Sinha 2003), H-like ions (Watanabe *et al.* 2003 - Fe, Mo; Alfaz Uddin *et al.* 2003 - He, Li, B, C, N, O, Ne, Fe; Bartlett & Stelbovics 2004 - Li, Be), He⁺ (Lepp, Stancil & Dalgarno 2002), He-like ions (Kuo & Huang 2001 - Li, B, C, N, Fe; Uddin *et al.* 2004b - Li, B, C, N, O, Ne, Fe), Li⁺ (Lepp, Stancil & Dalgarno 2002), Li²⁺ (Lepp, Stancil & Dalgarno 2002, Colgan, Pindzola & Robicheaux 2002), Li-like ions (Uddin *et al.* 2004a - C, N, O, Ne), Be ions (Colgan *et al.* 2003b - Be^{+−3+}), Be-like ions (Chang *et al.* 2004 - B, C, N, O, Ne, Al, Ar, Fe), C⁺ (Jha 2002), N⁺ (Jha 2002), O⁺ (Jha 2002), O⁴⁺ (Uddin *et al.* 2004a), O ions (Loch *et al.* 2003 - O^{+−4+}), Ne⁺ (Jha 2002), Ne⁶⁺ (Uddin *et al.* 2004a), Mg⁺ (Becker *et al.* 2004), Al ions (Aichele *et al.* 2001 - Al^{3−7+}), Ar ions (Zhang *et al.* 2002 - Ar^{4−11+}), Ti³⁺ (van Zoest *et al.* 2004), Ti¹¹⁺ (Qi *et al.* 2002a), Cr¹³⁺ (Qi *et al.* 2002b), and Kr ions (Khouilid *et al.* 2001 - Kr^{12−18+}; Loch *et al.* 2002 - Kr^{+−35+}; Beigman, Defrance & Vainshtein 2003a - Kr^{10−18+}; Beigman, Defrance & Vainshtein 2003b - Kr^{10−12,17,18+}).

Another important process is recombination for which a number of new works have appeared: He ions (Lepp, Stancil & Dalgarno 2002 - He^{+−2+}), He-like ions (Zhang & Sampson 2002 - O, Fe; O'Rourke *et al.* 2003 - Ti, Fe; Behar *et al.* 2004 - Ar, Fe), Li ions (Lepp, Stancil & Dalgarno 2002 - Li^{+−3+}; Colgan, Pindzola & Badnell 2004 - Be, B, C, N, O, Ne, Mg, Al, Si, P, S, Ar, Ti, Cr, Fe, Ni, Kr, Xe and others), Be⁺ (Mohamed *et al.* 2002, Schuch 2003), Be-like ions (Colgan *et al.* 2003a - B, C, O, N, Ne, Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Ni, Kr, Xe and others; Schnell *et al.* 2003 - F, Fe), B-like ions (Altun *et al.* 2004 - C, N, O, Ne, Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Ni, Kr, Xe and others), C³⁺ (Bureyeva *et al.* 2002b), C-like (Zatsarinny *et al.* 2004a - N, O, Ne, Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Co, Ni, Kr, Xe and others), N²⁺ (Kisielius & Storey 2002), N-like ions (Mitnik & Badnell 2004 - O, Ne, Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Ni, Kr, Xe and others), O⁵⁺ (Boehm *et al.* 2003, Murakami, Safronova & Kato 2002), O ions (Badnell *et al.* 2003 - O^{4−5+}), O-like ions (Chen 2002 - Mg, S, Si, Fe; Zatsarinny *et al.* 2003 - Ne, Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Co, Ni, Kr, Xe and others), Ne-like ions (Zatsarinny *et al.* 2004b - Mg, Al, Si, P, S, Ar, Ca, Ti, Cr, Fe, Co, Ni, Kr, Xe and others), Na⁸⁺ (Nikolic *et al.* 2004), Mg⁺ (Bureyeva *et al.* 2002b), Mg⁸⁺ (Schippers *et al.* 2004), Mg ions (Gu 2003a - Mg^{4−12+}; Gu 2003b - Mg^{2−11+}), Si¹⁴⁺ (Heerlein, Zwicknagel

& Toepffer 2002), Si ions (Gu 2003a - Si^{6-14+} ; Gu 2003b - Si^{4-13+}), S ions (Gu 2003a - S^{8-16+} ; Gu 2003b - S^{6-15+}), Ar ions (Gu 2003a - Ar^{10-18+} ; Gu 2003b - Ar^{8-17+}), Ca ions (Gu 2003a - Ca^{12-20+} ; Gu 2003b - Ca^{10-19+}), Ti^{20+} (O'Rourke *et al.* 2004), Fe^{17+} (Gorczyca, Badnell & Savin 2002, Zhang, Nahar & Pradhan 2001), Fe^{18+} (Savin *et al.* 2002), Fe^{23+} (Pindzola 2002), Fe ions (Gu 2003a - Fe^{18-26+} ; Gu 2003b - Fe^{16-25+} ; Gu 2003c - Fe^{16-23+} ; Dasgupta & Whitney 2004 - Fe^{24-25+}), Ni^{17+} (Fogle *et al.* 2003a, Fogle *et al.* 2003b), Ni ions (Gu 2003a - Ni^{20-28+} ; Gu 2003b - Ni^{18-27+} ; Dasgupta & Whitney 2004 - Ni^{26-27+}), Zn^{27+} (Bureyeva *et al.* 2002a, Bureyeva *et al.* 2002b), Kr^{34+} (Madzunkov *et al.* 2002), and Xe^{27+} (Yan, Li & Yao 2003).

3.4. Electron-Molecule Scattering

For molecules, new elastic scattering references have appeared as follows: H_2 (Lee & Mazon 2002), H_2O (Cho *et al.* 2004a, Faure, Gorfinkiel & Tennyson 2004), LiH (Antony *et al.* 2004), CH (Baluja & Msezane 2001), CH_4 (Ariyasinghe & Powers 2002, Ariyasinghe, Wijeratne & Palihawadana 2004), C_2H_2 (Ariyasinghe & Powers 2002), C_2H_4 (Ariyasinghe & Powers 2002, Panajotovic *et al.* 2003, Szmytkowski, Kwitnewski & Ptasinska-Denga 2003, Brescansin *et al.* 2004, Trevisan, Orel & Rescigno 2003), C_2H_6 (Ariyasinghe & Powers 2002, Maia & Bettega 2003), C_3H_4 (Nakano *et al.* 2002, Lopes & Bettega 2003), C_3H_6 (Curik & Gianturco 2002), C_4H_6 (Szmytkowski & Kwitnewski 2003, Lopes *et al.* 2004), C_6H_6 (Makochekanwa, Sueoka & Kimura 2003, Kimura, Makochekanwa & Sueoka 2004, Makochekanwa, Sueoka & Kimura 2004), CO (Blanco & Garcia 2003), CO_2 (Gianturco & Stoecklin 2001, Allan, M. 2002, Blanco & Garcia 2003), CS_2 (Allan, M. 2003), NO (Zhang *et al.* 2004), N_2 (Blanco & Garcia 2003), N_2O (Lee *et al.* 2002a, Akther *et al.* 2002, Allan & Skalicky 2003), O_2 (Garcia, Blanco & Williard 2001, Linert, Zubek & Zubek 2004), O_3 (de Pablos *et al.* 2002), OH (Sobrinho, Lozano & Lee 2004), OCS (Bettega, Lima & Ferreira 2004), SiH (Lee *et al.* 2002b), SiH_4 (Ariyasinghe, Wijerathna & Powers 2003), Si_2H_6 (Maia & Bettega 2003), PH_2 (Bettega & Lima 2004), PH_3 (Ariyasinghe, Wijerathna & Powers 2003, Szmytkowski *et al.* 2004), and SH (Baluja & Msezane 2002).

Regarding excitation, new references include: H_2 (Lee & Mazon 2002, Pigarov 2002, Celiberto, Capitelli & Laricchiuta 2002, Machado *et al.* 2001, Trevisan & Tennyson 2001, Wrkich *et al.* 2002, Curik & Carsky 2003, Harries, Hammond & Murray 2003, Liu *et al.* 2003, Horacek *et al.* 2004, da Costa, da Paixao & Lima 2004, Laricchiuta, Celiberto & Janev 2004), H_2O (Allan & Moreira 2002, Curik & Carsky 2003, Itikawa 2004, Faure, Gorfinkiel & Tennyson 2004), LiH (Antony *et al.* 2004), CH (Baluja & Msezane 2001), CH_4 (Nishimura & Gianturco 2002, Itikawa 2004, Joshipura *et al.* 2004), C_2H_4 (Panajotovic *et al.* 2003, Szmytkowski, Kwitnewski & Ptasinska-Denga 2003), C_2H_6 (Merz & Linder 2003a, Itikawa 2004), C_3H_4 (Nakano *et al.* 2002), C_4H_6 (Szmytkowski & Kwitnewski 2003), C_6H_6 (Makochekanwa, Sueoka & Kimura 2003), $\text{CH}_3\text{CH}_2\text{CH}_3$ (Merz & Linder 2003b), hydrocarbons (Janev & Reiter 2003 - CH , CH_2 , CH_3 , CH_4 , C_2H , C_2H_2 , C_2H_3 , C_2H_4 , C_2H_5 , C_2H_6 , C_3H , C_3H_2 , C_3H_3 , C_3H_4 , C_3H_5 , C_3H_6 , C_3H_7 , C_3H_8), CS_2 (Allan 2003, Michelin *et al.* 2003, Kroin *et al.* 2003), CO (Poparic, Vivic & Belic 2001, Kroin, Michelin & Lee 2001, Michelin *et al.* 2003), CO_2 (Rescigno *et al.* 2002, Green *et al.* 2002a, Rocha & Bielschowsky 2002, Allan 2002, McCurdy *et al.* 2003, Michelin *et al.* 2003, Kroin *et al.* 2003, Itikawa 2004, Vanroose *et al.* 2004), N_2 (Poparic, Vivic & Belic 2002, Feng, Sun & Morrison 2003), NO (Schappe, Edgell & Urban 2002), N_2O (Akther *et al.* 2002, Allan & Skalicky 2003), O_2 (Johnson & Kanik 2001, Green *et al.* 2002b, Terrell, Hansen & Ajello 2004), O_3 (de Pablos *et al.* 2002), OCS (Michelin *et al.* 2003, Kroin *et al.* 2003), SiH_4 (Ariyasinghe, Wijerathna & Powers 2003, Joshipura *et al.* 2004), PH_3 (Ariyasinghe, Wijerathna & Powers 2003), and SH (Baluja & Msezane 2002).

New work for dissociative processes consist of the following: H₂ (Harb, Kedzierski & McConkey 2000, Trevisan & Tennyson 2001, Krasheninnikov 2002, Pigarov 2002, Celiberto, Capitelli & Laricchiuta 2002, Fabrikant, Wadehra & Xu 2002, Horacek *et al.* 2004, Laricchiuta, Celiberto & Janev 2004), H₂O (Haxton *et al.* 2004), CH₄ (Luna *et al.* 2003), C₂H₄ (Szymtkowski, Kwitnewski & Ptasinska-Denga 2003), C₄H₆ (Szymtkowski & Kwitnewski 2003), C₆H₆ (Makochekeana, Sueoka & Kimura 2003), CH₃OH (Skalicky & Allan 2004), hydrocarbons (Janev & Reiter 2003 - CH, CH₂, CH₃, CH₄, C₂H, C₂H₂, C₂H₃, C₂H₄, C₂H₅, C₂H₆, C₃H, C₃H₂, C₃H₃, C₃H₄, C₃H₅, C₃H₆, C₃H₇, C₃H₈), CS₂ (Kedzierski 2002), NO (Allan 2004), N₂O (Allan & Skalicky 2003), and O₃ (de Pablos *et al.* 2002).

Research on molecular ionization have been performed on: H₂ (Hanel *et al.* 2002, Pigarov 2002, Celiberto, Capitelli & Laricchiuta 2002, Houamer *et al.* 2003, Mansouri *et al.* 2004, Liu & Shemansky 2004), H₂O (Champion, Hanssen & Hervieux 2002a, Hanel *et al.* 2002, Champion, Hanssen & Hervieux 2002b, Vinodkumar *et al.* 2003 - crystalline ice; Champion, Hanssen & Hervieux 2004), H₂S (Lindsay, Rejoub & Stebbings 2003), B₂H₆ (Basner, Schmidt & Becker 2003), CH₄ (Stano *et al.* 2003, Luna *et al.* 2003, Joshipura *et al.* 2004, Champion, Hanssen & Hervieux 2004), C₂H₄ (Szymtkowski, Kwitnewski & Ptasinska-Denga 2003), C₆H₆ (Hanel *et al.* 2002, Makochekeana, Sueoka & Kimura 2003), CH₃COCOCH₃ (Takahashi *et al.* 2003), hydrocarbons (Janev & Reiter 2003 - CH, CH₂, CH₃, CH₄, C₂H, C₂H₂, C₂H₃, C₂H₄, C₂H₅, C₂H₆, C₃H, C₃H₂, C₃H₃, C₃H₄, C₃H₅, C₃H₆, C₃H₇, C₃H₈), CO (Hudson, Vallance & Harland 2004), CO₂ (Hudson, Vallance & Harland 2004), CS₂ (Lindsay, Rejoub & Stebbings 2003, Hudson, Vallance & Harland 2004), NH₃ (Champion, Hanssen & Hervieux 2004), N₂O (Lindsay, Rejoub & Stebbings 2003), NO₂ (Jiao, DeJoseph & Garscadden 2002), O₂ (Johnson & Kanik 2001, Joshipura, Antony & Vinodkumar 2002), O₃ (Joshipura, Antony & Vinodkumar 2002), O₄ (Joshipura, Antony & Vinodkumar 2002), OCS (Hudson, Vallance & Harland 2004), OHCCHO (Takahashi *et al.* 2003), SiH₃ (Ariyasinghe, Wijerathna & Powers 2003), SiH₄ (Joshipura *et al.* 2004), and PH₃ (Ariyasinghe, Wijerathna & Powers 2003).

Andersen, Herber & Zajfman (2004) have studied negative ion formation from C₂.

3.5. Electron-Molecular-Ion Scattering

New elastic scattering results exist for H₃⁺ and H₃O⁺ (Faure & Tennyson 2002a).

For excitation, studies have been conducted for: H₂⁺ (Pigarov 2002), H₃⁺ (Faure & Tennyson 2002a, Faure & Tennyson 2002b, Gorfinkiel & Tennyson 2004), H₃O⁺ (Faure & Tennyson 2002a, Faure & Tennyson 2002b), and hydrocarbon ions (Janev & Reiter 2003 - CH⁺, CH₂⁺, CH₃⁺, CH₄⁺, C₂H⁺, C₂H₂⁺, C₂H₃⁺, C₂H₄⁺, C₂H₅⁺, C₂H₆⁺, C₃H⁺, C₃H₂⁺, C₃H₃⁺, C₃H₄⁺, C₃H₅⁺, C₃H₆⁺, C₃H₇⁺, C₃H₈⁺).

References on dissociative processes have appeared for: H₂⁺ (Neau *et al.* 2002, Krasheninnikov 2002, Pigarov 2002, Takagi 2002, Strasser *et al.* 2002b, Florescu *et al.* 2003, Al-Khalili *et al.* 2003, Abdellahi El Ghazaly *et al.* 2004), H₃⁺ (Krasheninnikov 2002, Glosik *et al.* 2001, Strasser *et al.* 2002a, McCall *et al.* 2004, Royal, Larson & Orel 2004, Gorfinkiel & Tennyson 2004, Kalhori *et al.* 2004), HeH⁺ (Royal, Larson & Orel 2004, Takagi 2004), H₂O⁺ (Thomas *et al.* 2002), CH⁺ (Bannister *et al.* 2003), CH₄⁺ (Janev 2002), C₂H₂⁺ (Derkatch, Minaev & Larsson 2003), C₂H₄⁺ (Janev 2002), ₂H₆⁺ (Janev 2002), C₃H₈⁺ (Janev 2002), CO₂⁺ (Bahati *et al.* 2001a, Seiersen *et al.* 2003), N₂⁺ (Bahati, E. M. *et al.* 2001b), and SO₂⁺ (Geppert *et al.* 2004).

New reports of results for ionization include: H₂⁺ (Serov *et al.* 2002), H₃⁺ (Gorfinkiel & Tennyson 2004), hydrocarbon ions (Janev & Reiter 2003 - CH⁺, CH₂⁺, CH₃⁺, CH₄⁺, C₂H⁺, C₂H₂⁺, C₂H₃⁺, C₂H₄⁺, C₂H₅⁺, C₂H₆⁺, C₃H⁺, C₃H₂⁺, C₃H₃⁺, C₃H₄⁺, C₃H₅⁺, C₃H₆⁺,

$C_3H_7^+$, $C_3H_8^+$, CO_2^+ (Bahati *et al.* 2001a, Deutsch *et al.* 2002), and N_2^+ (Deutsch *et al.* 2002, Bahati *et al.* 2001b).

Finally, recombination of electrons with molecular ions have been studied for: H_2^+ (Neau *et al.* 2002, Krasheninnikov 2002, Pigarov 2002, Takagi 2002, Florescu *et al.* 2003, Ngassam *et al.* 2003, Al-Khalili *et al.* 2003), H_3^+ (Glosik *et al.* 2001, Strasser *et al.* 2002a, Strasser *et al.* 2002b, Kokouline & Greene 2003a, 2003b, McCall *et al.* 2004, Royal, Larson & Orel 2004), H_2O^+ (Thomas *et al.* 2002), HeH^+ (Royal, Larson & Orel 2004, Takagi 2004), hydrocarbon molecular ions (Janev 2002 - CH_4^+ , $C_2H_4^+$, $C_2H_6^+$, $C_3H_8^+$; Derkatch, Minaev & Larsson 2003 - $C_2H_2^+$), CO_2^+ (Seiersen *et al.* 2003), NH_4^+ (Ojekull *et al.* 2004), N_2H^+ (Geppert *et al.* 2004a), and SO_2^+ (Geppert *et al.* 2004b).

3.6. Ion-Atom and Atom-Atom Collisions

Charge transfer plays an important role in a variety of environments and therefore has seen a substantial amount of activity over the report period. Studies for collisions on H include: H^+ (Cabrera-Trujillo *et al.* 2002a, Celiberto *et al.* 2002, Killian *et al.* 2004, Krstić *et al.* 2004), He^{2+} (Le *et al.* 2004), Li^{+3+} (Purkait 2003), Li^{3+} and Ne^{10+} (Errea *et al.* 2004b), B^{2+} (Turner *et al.* 2003), C^{4+} (Liu *et al.* 2003), $C^{4,5+}$, $N^{5,6+}$, and $O^{6,7+}$ (Kearns *et al.* 2003), N^+ (Lin *et al.* 2005), N^{2+} (Barragan *et al.* 2004), N^{4+} (Cabrera-Trujillo *et al.* 2002c), N^{5+} (Kearns *et al.* 2002), O^+ (Spirko *et al.* 2003), O^{2+} (Cabello *et al.* 2003), O^{3+} (Wang *et al.* 2003), O^{8+} and Ar^{8+} (Edgu-Fry *et al.* 2004, Lee *et al.* 2004), Ne^{2+} (Mroczkowski *et al.* 2003), Ne^{3+} (Rejoub *et al.* 2004), and Ne^{4+} (Havener *et al.* 2004). Collisions of neutral species with protons include: He^* (Chibisov *et al.* 2002), N (Lin *et al.* 2005), Na (Watanabe *et al.* 2002, Le *et al.* 2003), S (Zhao *et al.* 2005a), Ar (Kirschner *et al.* 2004), and K (Watanabe *et al.* 2002, Hayakawa *et al.* 2004).

Neutral helium is also an important target for which studies have considered the incident ions: H^+ (Minami *et al.* 2004), $Be^{3,4+}$ (Shimakura *et al.* 2003), C^{2+} (Gao & Kwong 2003), C^{2-6+} , N^{2-6+} , O^{2-6+} (Ishii *et al.* 2004), O^+ (Lindsay & Stebbings 2003, Zhao *et al.* 2005b), O^{5+} (Sobocinski *et al.* 2003), O^{6+} and Ne^{8+} (Bordenave-Montesquieu *et al.* 2003), O^{7+} (Shevelko *et al.* 2004), Ne^{2+} (Imai *et al.* 2003), Ne^{4+} (Kamber *et al.* 2003), Ne^{10+} (Rigazio *et al.* 2002, Ali *et al.* 2005), S^{2+} (Zhao *et al.* 2005c), S^{4+} (Wang *et al.* 2002), Ar^{9+} (Bliman *et al.* 2002), and Fe^{5-13+} (Čadež *et al.* 2003). The reverse process through radiative charge transfer has been considered for $O + He^+$ (Zhao *et al.* 2004). Some relevant symmetric charge transfer studies were done for $N^+ + N$ and $O^+ + O$ (Eletskii *et al.* 2004). On-line databases of charge transfer data include the National Institute for Fusion Science (NIFS) Charge Transfer Database Chart (2005) and the ORNL/UGA Charge Transfer Database for Astrophysics (2005) sites.

Elastic scattering and spin exchange have been studied for $H^+ + H$ by Krstić *et al.* (2004) and Glassgold *et al.* (2005) while Zygelman *et al.* (2003) reported new spin-exchange calculations for $H + H$. Chung & Dalgarno (2002) studied diffusion of H in He and He in H.

Molecules can be formed by collisions of atoms through radiative association. Bennett *et al.* (2003) studied the role of quasi-bound states in the formation of LiH. Atom collisions can also result in changes in internal energy and recent work includes: Li with H (Belyaev & Barklem 2003), He^* with He (Vrinceanu & Sadeghpour 2002), and C and S with He (Le Picard *et al.* 2002).

3.7. Ion-, Atom-, and Molecule-Molecule Collisions

In photoionized environments, multiply charged ions may coexist with neutral molecules. Examples include x-ray ionized regions and solar wind interactions with cometary gas. In these environments charge transfer plays an important role. Recent studies of

ion-molecule charge transfer include H^+ (Cabrera-Trujilla *et al.* 2002b, Savin *et al.* 2004), H^+ and D^+ (Kuskabe *et al.* 2004), He^{2+} (Errea *et al.* 2003), C^{2+} (Gao & Kwong 2003), C^{4+} (Konnai *et al.* 2003), C^{4-5+} , N^{5-6+} , and O^{6-7+} (Kearns *et al.* 2003), N^{5+} (Kerns *et al.* 2002, Errea *et al.* 2004a), O^+ (Pichl *et al.* 2003), O^{3+} (Wang *et al.* 2004), O^{6+} (Bordenave-Montesquieu *et al.* 2003), O^{8+} and Ar^{8+} (Edgu-Fry *et al.* 2004), S^{2+} (Chen *et al.* 2003), and Fe^{3+} (Gao *et al.* 2003) with H_2 ; C^{2+} (Gao & Kwong 2003), C^{3-4+} (Gao & Kwong 2002), and S^{2+} (Chen *et al.* 2003) with CO; H^+ (Cabrera-Trujillo *et al.* 2002d), C^{2+} (Gao & Kwong 2003), S^{2+} (Chen *et al.* 2003), and Fe^{3+} (Gae *et al.* 2003) with N_2 ; He^{2+} with H_2O and CO_2 (Abu-Haija *et al.* 2003); and H^+ with CH_2 (Suno *et al.* 2004).

For applications to x-ray emission from comets a number of investigations have considered a range of highly charged ions on various molecular targets including $Ne^{+,3,5,7,9+}$ with H_2O (Pesic *et al.* 2004); Ne^{10+} with H_2 , H_2O , and CO_2 (Rigazio *et al.* 2002); and Ne^{10+} with CO and CO_2 (Ali *et al.* 2005). Also, see Krasnopolsky *et al.* (2004) for a review of cometary x-ray relevant collision data.

In some environments, advances in modeling require vibrationally-resolved charge transfer and dissociation data. Such data are generally not available, but some studies have been performed for $H^+ + H_2$ and $H + H_2^+$ (Krstić & Janev 2003), $O^{3+} + H_2$ (Wang *et al.* 2004), and $O^{3+} + HD$ (Stancil *et al.* 2004).

In low ionization environments, excited rovibrational states of molecules are formed through collisional excitation by atom and molecule impact. Investigations have been performed for excitation of H_2 by H (Mielke *et al.* 2003), by He (Lee *et al.* 2005), by H_2 (Ceballos *et al.* 2002, Lin & Guo 2002), and by Li^+ (Roeggen *et al.* 2002); CO by H (Yang *et al.* 2005a), by He (Krems, *et al.* 2002, Carty *et al.* 2004, Smith *et al.* 2004, Yang *et al.* 2005b), and by H^+ (Kumar & Kumar 2004); N_2 by He (Stoeklin *et al.* 2002); F_2 by He (Stoeklin *et al.* 2003); SiO by H (Palov *et al.* 2002); CaH by He (Krems *et al.* 2003); H_2O by H_2 (Dubernet & Grosjean 2002, Grosjean *et al.* 2003, Weisenfeld *et al.* 2003); N_2 by N_2 (Ramos *et al.* 2002); N_2 by CO (Cacciatore *et al.* 2004); CO by CO (Billings *et al.* 2003); and CH_3OH by He (Flower and Davis 2004). A useful online database of rovibrational collisional excitation data, BASECOL, can be found at: <http://amdpo.obspm.fr/basecol/>.

Elastic scattering data for vibrationally-excited molecules have been presented by Krstić & Schultz (2003) for $H^+ + H_2$ and $H + H_2^+$ collisions. An online database can be found at: <http://cfadc.phy.ornl.gov/elastic/homeph2.html>.

3.8. Reactive Scattering and Chemistry

Due to space limitations, we cannot review the many advances in reactive scattering and chemical processes relevant to astrophysics. However, some noteworthy and relevant studies include OH formation in $O + H_2$ collisions (Baunstein *et al.* 2004, Balakrishnan 2004, Sultanov & Balakrishnan 2004), CO_2 formation in $OH + CO$ collisions (Valero & Kroes 2004), OH formation in $H + H_2O$ collisions (Zhang *et al.* 2002), and H_2 formation in $LiH + H$ collisions (Kim *et al.* 2003).

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4. Working Group on Line Broadening

PRESIDENTS: N.F. Allard and G. Peach

Two conferences held in 2004 and 2005 have been devoted to the subject of Spectral Line Shapes. The 17th International Conference on Spectral Line Shapes (ICSLS) was held at the Université Pierre et Marie Curie in Paris (France) in 2004; the proceedings have been published by the Editions Frontier group and include a special section on astrophysical applications. The 5th Serbian Conference on Spectral Line Shapes in

Astrophysics (SCSLSA) was held in Vršac in 2005 and the proceedings have been published in *Memorie della Supplementi degli Società Astronomica Italiana* (Mem. S.A.It.).

In the following report, we select experimental and theoretical work that may be of interest for astrophysics.

4.1. *Stark broadening*

The Critical Review of Selected Data on Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms for the period 1989-2000, see Konjević *et al.* (2002), contains tables where measured values are listed and compared with semi-classical calculations. The Bibliography of Line Shapes and Shifts contains more recent data, see section 3 on Databases. There are also several papers on Stark broadening and plasma-induced line shifts among the articles published as a tribute to Charles Hooper under the collective title Radiative Properties of Hot Dense Matter (Lee 2003). An overview of the role of the plasma micro field in the Stark broadening of spectral lines has been presented by Demura (2004) and Demura and Gilles (2004). These articles contain many useful references.

A short review of the French-Serbian collaboration on theoretical calculations of Stark broadening of spectral line shapes for non-hydrogenic atoms within the framework of the semi-classical approach has been presented by Dimitrijević and Sahal-Bréchet (2004).

Developments in line broadening theory

Alexiou and Poquérusse (2005) and Poquérusse and Alexiou (2005) have extended standard semi-classical impact theory for hydrogen and hydrogenic ions to include penetrating collisions. Alexiou and Lee (2005) have tested this theory against full quantum mechanical calculations for hydrogen and have found that the difference between the two is much reduced. Bouguettaia *et al.* (2005) have re-derived results for Lyman- α using a path integral formalism that treats the electron and proton perturbers on the same basis.

Elabidi *et al.* (2004b) have obtained a new quantum-mechanical formula for the electron impact width and shift of isolated lines using intermediate coupling and a quantum kinetic theory approach to the line broadening of isolated lines with stationary non-equilibrium level populations has been developed by Iglesias (2005).

Isolated lines

The term ‘isolated lines’ means lines between atomic levels that are sufficiently separated from the other atomic levels to enable the Stark effect to be treated within perturbation theory (second-order Stark effect). The line broadening and shift is dominated in this case by the interaction with the plasma electrons. Recent theoretical results have been obtained for lines of Ag I (Dimitrijević and Sahal-Bréchet 2003), Be III (Dimitrijević *et al.* 2003), O II and C II (Mahmoudi *et al.* 2004a, 2004b, 2005), Tl II (Milovanović 2005) and Cu III and Zn III (Simić *et al.* 2005).

Stark broadening of lines of He I, Mg I and Ar I for a perturber density of 10^{16} cm^{-3} and for temperatures between 2,500 K and 50,000 K have been investigated by Zmerli *et al.* (2005). Theoretical results have also been obtained for lines of Ne I (Milosavljević and Djenize 2002b), (Milosavljević *et al.* 2004), Ar I (Valognes *et al.* 2004, 2005) and Kr I (Milosavljević *et al.* 2003), (Milosavljević 2005). Calculations of line widths for Ar I (Ben Nessib and Sahal-Bréchet 2004) are compared with the experimental values of Milosavljević and Djenize (2003a, 2003b, 2003c) and Nikolić *et al.* (2004). Cadwell and Hüwel (2004) have determined Stark-broadening parameters for 12 Ar I lines from time-resolved emission spectra with an estimated accuracy of 20%.

Stark broadening parameters for Cd I have been calculated by (Simić 2005) for 11 singlets and 13 triplets in the ultraviolet and visible spectral region and 24 triplets in the infrared, for temperatures between 2,500 K and 50,000 K, and for a perturber density of 10^{16} cm^{-3} . Moreover line widths have been obtained within the modified semi-empirical approach for 10 F III multiplets, for temperatures 10,000 K–300,000 K and for a perturber density of 10^{17} cm^{-3} . Dimitrijević *et al.* (2005) have used the impact approximation to calculate line widths and shifts for the $4p^7 \text{ P}^0\text{-}4d^7 \text{ D}$ transitions in Cr I broadened by electrons, protons and ionized helium.

Most of these results have been obtained by using semi-classical theory which provides a powerful tool for the rapid calculation of line widths and shifts.

Quantum-mechanical Stark broadening calculations for lines of Ne VII and Ne VIII which are in intermediate coupling have been carried out by Elabidi *et al.* (2004a, 2005). Hydrogen-like and helium-like ions of C, Si and Ar have been studied by Stambulchik and Maron (2005) using a numerical simulation of the plasma particle motion and find that ion dynamics is very important for these cases.

Hydrogen lines

The occupation probability method (OPM) is normally applied to the matching of discrete and continuous radiative spectra in dense hydrogenic plasmas (Vitel *et al.* 2004). An alternative method that removes the matching problem has been developed by D'yachkov (2004) and the results obtained are in good agreement with experimental data.

The Stark broadening of the Radio Recombination Lines (RRLs) of Hydrogen observed from galactic H II regions is controlled by inelastic collisions with charged particles. Gavrilenko and Oks (2004) have presented a method of calculating both the cross sections of such collisions and the Stark broadening of RRLs based on the classical-trajectory Monte Carlo approach.

For lines of hydrogen in the visible and ultraviolet, measurements of widths and shifts for the Balmer α and β lines in a laser-induced plasma have been made by Parigger *et al.* (2003, 2004). Stark widths and shifts of the $\text{H}\alpha$ line measured in a flash tube plasma have been compared with theoretical results by Griem and Halenka (2004) and Flih *et al.* (2003, 2004). Also a theoretical study of the Lyman γ line profile of atomic hydrogen perturbed by collisions with protons is reported by Allard *et al.* (2004).

Spectroscopic diagnostics of warm dense matter are presented by Astapenko *et al.* (2004).

Neutral Helium lines

Stark broadening calculations for the spectral line of neutral helium at 6678 Å formed in a non-ideal plasma have been performed by Ben Chaoucha *et al.* (2004). Stark line profiles for He I lines emitted by dense plasmas have also been calculated by Gigosos *et al.* (2004) and Ozmar *et al.* (2004) and compared to the experimental results of Milosavljević and

Djenize (2003d). Calculations have also been carried out for lines of He I by Milosavljević and Djenize (2002a), Li and You (2002) and Bardet *et al.* (2003).

4.2. Broadening by neutral atoms and molecules

A collection of papers concerning the status of the molecular spectroscopic database, HITRAN 2000, has been published by Rothman *et al.* (2003) and this has recently been updated for the current version HITRAN 2004 by Rothman *et al.* (2005). These reviews contain papers specific to line broadening and shift phenomena in molecules.

An overview of state-of-the-art simulations of cool stellar atmospheres using the code PHOENIX was presented by Hauschildt and Baron (2005) and Homeier (2005) at the SCSLSA meeting. Molecules are the dominant opacity source and the resonance lines of Na and K have line wings that are particularly strong features of these spectra. The main difficulty is the lack of much realistic experimental or theoretical data for collision broadening by the dominant perturbers in these atmospheres, H₂ and He. The assumption of Van der Waals broadening gives at best only crude estimates for the line broadening parameters.

Developments in line shape theory

Beaud and Knopp (2003) have developed a method of scaling rotationally inelastic collisions with an effective angular momentum parameter and applying it to collision-induced intra-molecular rotational energy transfer. Excellent agreement with experiment has been achieved for the CO–CO, N₂–N₂ and N₂–He systems. Wang (2004) has produced a refined version of the non-perturbative pressure-broadening theory of Neilson and Gordon and has obtained good agreement for CO lines in the fundamental band broadened by Ar.

Broadening of atomic lines

Some theoretical work has been published in the period 2002–2005 and the transitions with the perturbing atoms or molecules are listed below.

Li far-wing profile of the 2s–2p resonance line broadened by He (Zhu *et al.* 2005).

Na far-wing line profiles for the 3s–3p resonance line broadened by He, Ar and Xe Chung *et al.* (2002).

Na and K full line profiles including far line wings of the resonance lines broadened by H and H₂ (Allard *et al.* 2003).

Na and K far-wing line profiles of the resonance lines broadened by H₂ and He (Burrows and Volobuyev 2003).

Na line broadening and mixing in the 3p–3d transition broadened by H (Sanchez-Fortún Stoker and Dickinson 2003).

Na line widths for the 3s–3p and 3d–4p transitions broadened by He (Peach *et al.* 2005).

Broadening and shift of molecular lines

Much more experimental data has been published since the last report was prepared. The molecules are listed below with their perturbing atomic or molecular species.

D₂ collision-induced absorption in the fundamental band in D₂–N₂ and D₂–O₂ mixtures (Varghese *et al.* 2004).

HCN lines in the 2ν₂ region broadened and shifted by HCN and air (Devi *et al.* 2004).

HNO₃ millimeter-wave transitions broadened by N₂ and O₂ (Colmont *et al.* 2003).

H₂O lines in the 26000–13000 cm^{−1} region broadened by H₂O and N₂ (Coheur *et al.* 2002).

H₂O 183 GHz line broadened and shifted by N₂, O₂ and air (Tretyakov 2003).
H₂O self-broadened pure rotational lines (Podobedov *et al.* 2004).
H₂O lines in the ν_2 band broadened by air (Wagner *et al.* 2005).
H₂O lines in the 1.39 μ m region broadened by N₂, O₂ and air (Durry *et al.* 2005).
H₂S lines in the ν_2 band broadened and shifted by H₂, D₂, N₂, O₂ and CO₂ (Kissel *et al.* 2002).
HCl $J = 1 - 0$ rotational transition broadened and shifted by N₂, O₂ and Ar (Morino and Yamada 2005).
CH₄ two lines of the $2\nu_3$ band broadened by N₂, O₂, He and Ar (Dufour *et al.* 2003).
CO $J = 5 - 4$ transition at 576 GHz broadened and shifted by CO, N₂ and O₂ (Markov *et al.* 2002) and by He, Ne, Ar, Kr and Xe (Yamada and Abe 2003).
CO $R(7)$ and $R(7)$ transitions in the fundamental band broadened by Ar (Mantz *et al.* 2003).
CO second overtone band broadened and shifted by CO and air (Sung and Varanasi 2004).
CO₂ lines in the 1.6 μ m region broadened by N₂ and O₂ (Pouchet *et al.* 2004).
CO₂ and OCO self-broadened lines near 2.04mm (Le Barbu *et al.* 2005).
CF₄ lines in the ν_4 band broadened by He, N₂ and Ar (Domanskaya *et al.* 2004).
CF₃CFH₂ rotational lines broadened by CF₃CFH₂, N₂ and O₂ (Cazzoli *et al.* 2004).
NH₃ 134 rovibrational transitions in the ν_4 and $2\nu_2$ bands broadened by H₂ and N₂ (Nouri *et al.* 2004).
N₂O millimeter lines broadened by N₂ and O₂ (Rohart *et al.* 2003).
O₂ 60-GHz band and single line at 118.75 GHz broadened by N₂, O₂, He, Ne, Ar, H₂O, CO and CO₂ (Golubiatnikov *et al.* 2003).
O₂ single line at 118.75 GHz broadened and shifted by O₂ and air (Tretyakov *et al.* 2004).
O₂A-band broadened by He, Ne, Ar, Kr and Xe (Pope *et al.* 2004).
O₂-O₂ collision-induced resonances at 477nm and 577nm (Sneep *et al.* 2005).
O₃ submillimeter-wave lines broadened by N₂, O₂ and air (Yamada and Amano 2005).
O₃ millimeter-wave lines broadened by N₂, O₂ and air (Colmont *et al.* 2005).
PH₃ ν_2 and ν_4 bands broadened by H₂, He and Ar (Bouanich *et al.* 2004), (Salem *et al.* 2004, 2005).
Theoretical results obtained during the period 2002-2005 are listed below.
H₂O effects of vibration on lines broadened and shifted by N₂ (Gamache and Hartmann 2004).
H₂O 11 vibrational bands in the range 3.2–17.76 μ m broadened by N₂, O₂ and air (Gamache 2005).
CH₃D lines in the ν_2 band broadened by He (Féjard *et al.* 2003).
CO lines in the fundamental and first two overtone bands broadened and shifted by H₂ (Bouanich and Predoi-Cross 2005).

4.3. Databases

A 'virtual observatory' has been developed for astronomers to give immediate access to data archives, databases, reference surveys and information services anywhere in the world, see:

cdsarc.u-strasbg.fr,

and the latest version of the database High resolution Transmission, HITRAN 2004, can be found at:

<http://www.hitran.com>.

The current version of the database Gestion et Etude des Informations Spectroscopiques Atmosphériques (GEISA-03) is at:

<http://ara.lmd.polytechnique.fr>,

and the Spherical Top data System (STDS), for spherical top molecules is at:

<http://www.u-bourgogne.fr/LPUB/sTDS.html>.

The National Institute for Standards and Technology (NIST) maintains a database at:

<http://www.physics.nist.gov/PhysRefData>,

which contains the Bibliography on Atomic Line Shapes and Shifts up to 1999 and the database at the Observatoire de Paris,

<http://amrel.obspm.fr/balss>,

contains the Bibliography up to 2003. The Vienna Atomic Line Database (VALD) can be found at:

<http://www.astro.univie.ac.at/~vald>,

and the Belgrade database at:

<http://www.aob.bg.yu/BELDATA>.

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