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Div. XII / Commission 14 WG	**Atomic Data**
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TRIENNIAL REPORT 2006-2009

1. Introduction

The main purpose of Commission 14 is to foster interactions between the astronomical community and those conducting research on atoms, molecules and solid state particles. This triennial report for Commission 14 covers the topics Atomic Data and Solids and Their Surfaces. Before doing so, we highlight the meetings sponsored by the Commission.

2. Sponsored meetings within the past triennium

Past meetings:

- IAU Symposium No. 234, *Planetary nebula in our galaxy and beyond*, April 2006, Waikoloa Beqach, HI USA
- IAU Symposium No. 251, *Organic matter in space*, February 2008, Hong Kong, China

Future Meetings (next GA):

- Special Session, *IR and sub-mm spectroscopy: A new tool for stellar evolution* (co-sponsor)
- *Eta Carinae and interacting massive binaries* (supported)
- *Progress in understanding the physics of Ap and related stars* (supported)

Steven R. Federman
president of the Commission

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3. Energy Levels, Wavelengths, Line Classifications, and Line Structure

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. References including experimental data on line structure, hyperfine structure (HFS) or isotope structure (IS) are also included.

Li I [181], **C I** [136, 247], **N I** HFS,IS [109], **Ne II** IS [182, 125, 128], **Ne III** [182, 129], **Ne IV** [92], **Mg I** IS [212], **Al VI** HFS [45], **S VII-S XIV** [146], **K II** [193], **Sc I** HFS [135], **Cr I** IS [87], **Mn I** HFS [39], **Mn II** HFS [40], **Fe XV - Fe XIX** [161], **Kr I** [214], **Sr I** HFS,IS [53], **Nb I** HFS [133, 134 **Cs I** HFS [55], **La I** HFS [22, 89], **La II** HFS [220], **Pr I** HFS [88], **Pr II** HFS [90, 91], **Nd II** HFS,IS [122, 157, 198], **Nd III** [199], **Nd IV** [256, 257], **Sm II** HFS [156], **Eu III** [258], **Gd I** IS [107], **Tm I** HFS [21], **Tm IV** [165], **Yb I** HFS [56], **Yb III** [183], **Hf II** [155], **Ta I** HFS [106], **Pb I** IS [252].

The references for elements heavier than Ni (Z>28) are limited to the first three or four spectra only, these data being of most 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 data in a number of the references above include and/or supersede all or most of the previously data for the indicated spectrum.

Current analyses of high-resolution laboratory spectra (energy levels, wavelengths) is ongoing at Lund, Sweden (transition and rare-earth elements), London, UK (iron-group elements), NIST, USA (transition and rare-earth elements, HFS), Troitsk, Russia (heavy elements), and Meudon & Orsay, France (transition and rare-earth elements, theory).

4. Wavelength Standards

Ritz wavelengths of forbidden lines of [Fe II], [Ti II], and [Cr II] have been measured using energy levels derived using Fourier transform spectroscopy (FTS) [10]. Accurate wavelengths of spectral lines in iron-group elements have been measured using FTS with uncertainties of around 10^{-5} nm [11]. The most accurate frequency standards are now being measured using laser spectroscopy with calibration from a laser frequency comb. Frequencies with uncertainties of less than 1 MHz have been measured for **H I** [99], **Mg I** [212], **K I** [73], **Rb I** [160], **Sr I** [53], **Cs I** [77, 94], and **In II** [250] using this technique.

Wavelengths of spectral lines from a Th/Ar hollow cathode lamp suitable for calibration of astronomical spectrographs have been published by various authors [117, 154, 172]. A correction to the wavelength scale of Ar I published by Whaling et al. in 2002 [253] is given in [213].

5. Transition Probabilities

The references listed in section 9 are for the period 2005 – 2008. The transition-probability data in these references were obtained by both theoretical and experimental methods. The references for elements heavier than Ni (Z>28) are limited to the first three or four spectra only. All papers contain a significant amount of numerical data, normally for more than ten spectral lines. Extensive results of atomic structure calculations are also given in reference [81].

6. Larger Compilations, Reviews, Conference Proceedings

The following compilations on wavelengths and energy levels have been published by the Atomic Spectroscopy group at NIST: **Be II** [124], **B I** [130], **Ne II** [128], **Ne III** [129], **Ne VII** [126], **Ne VIII** [127], **K I-K XIX** [217], **Ga I - Ga XXXI** [227], **Kr I - Kr XXXVI** [211], **Rb I - Rb XXXVII** [215], **W I** [131], **W II** [131], **Hg I** [210], **Fr I** [216] In addition to these comprehensive compilations, the *Handbook of basic atomic spectroscopic data* [218] contains a selection of the strongest spectral lines of neutral and singly-ionized atoms of all elements from hydrogen to einsteinium. Compilations by other groups include **He I** [69, 169], **B II** [201], and a compilation of coronal lines [76].

The following additional major compilations of transition probability data have been published during the latest three year period: **Na-like to Ar-like sequences** [81], ^{4}**He I** [70], **Fe I** and **Fe II** [85], **C I, C II, N I** and **N II** [254], (Erratum: [255]). Additional data can be found in *NIST Atomic Transition Probabilities,*86.

A number of papers on atomic spectroscopic data are included in proceedings of the *Ninth International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, held in Lund, Sweden, August 2007. Invited papers are published in the Physica Scripta T Series (Wahlgren, Wiese & Beiersdorfer 2008) and poster papers are published in the on-line open access Journal of Physics: Conference Series (Wahlgren, Wiese & Beiersdorfer 2008).

Papers on astrophysical data needs are included in the proceedings from the International Conferences on Atomic and Molecular Data *ICAMDATA* (Meudon, France, October 2006; Beijing, China, October 2008) and the fifteenth international conference on atomic processes in plasmas (NIST, March 2007). These proceedings contain review papers as well as descriptions of atomic and molecular databases.

7. Atomic Spectroscopic Data on the Internet

The following databases of atomic spectra are available at NIST. Most of these have received major updates since the last trienniel report.

Atomic Spectra Database:
`http://physics.nist.gov:/PhysRefData/ASD/index.html`

Handbook of Basic Atomic Spectroscopic Data:
`http://physics.nist.gov/PhysRefData/Handbook/index.html`

Energy Levels of Hydrogen and Deuterium:
`http://physics.nist.gov/PhysRefData/HDEL/index.html`

Ground Levels and Ionization Energies for the Neutral Atoms:
`http://physics.nist.gov/PhysRefData/IonEnergy/ionEnergy.html`

Spectral Data for the Chandra X-ray Observatory:
`http://physics.nist.gov/PhysRefData/Chandra/index.html`

NIST Atomic Spectra Bibliographic Databases:
`http://physics.nist.gov/PhysRefData/ASBib1/index.html`

Consists of three databases of publications on atomic transition probabilities, atomic energy levels and spectra, and atomic spectral line broadening. All three are updated on a frequent basis.

Additional on-line databases including significant quantities of atomic data include:

The MCHF/MCDHF Collection on the Web (C.Froese Fischer *et al.*) at http://www.vuse.vanderbilt.edu/~cff/mchf_collection/ contains results of multi-configuration Hartree-Fock (MCHF) or multi-configuration Dirac-Hartree-Fock (MCDHF) calculations for hydrogen and Li-like through Ar-like ions, mainly for $Z \leqslant 30$. Data for fine-structure transitions are included.

The TOPbase and Opacity Projects include transition probability and oscillator strength data for astrophysically abundant ions ($Z \leqslant 26$). A database is available at http://vizier.u-strasbg.fr/topbase/topbase.html. Revised opacities for stellar astrophysics have been made available during the current reporting period.

The D.R.E.A.M. database (Database on Rare Earths at Mons University) (w3.umh.ac.be/ astro/dream.shtml) continues to be a relevant source of data for wavelengths, energy levels, oscillator strengths and radiative lifetimes for neutral, singly and doubly-ionized rare earth elements. New data have not been added to this database during the past three years.

CHIANTI, an atomic database for spectroscopic diagnostics of astrophysical plasmas (http://wwwsolar.nrl.navy.mil/chianti.html), contains atomic data and programs for computing spectra from astrophysical plasmas, with the emphasis on highly-ionized atoms. During the current reporting period additions to the database (version 5) include new physical processes and atomic data.

The Vienna Atomic Line Database (VALD) web site (http://ams.astro.univie.ac.at/ vald/) allows users to extract atomic line data from a compilation of numerous sources according to element or presence in stellar spectra.

The bibl database is a comprehensive bibliographic database on atomic spectroscopy with a search engine on various atomic parameters is available at the Institute of Spectroscopy, Troitsk, (http://das101.isan.troitsk.ru/bibl.htm).

8. List of References

The references are identified by a running number. This refers to the general reference list at the end of this report, where the literature is ordered alphabetically according to the first author. Each reference contains one or more code letters indicating the method applied by the authors, defined as follows:

THEORETICAL METHODS:

Q: quantum mechanical calculations.

QF: quantum mechanical calculations of forbidden lines.

EXPERIMENTAL METHODS:

El: Energy levels.

HFS: Hyperfine structure.

L: Lifetimes.

TE: Emission transition probabilities.

Wl: Wavelengths.

IS: Isotope structure.

M: Miscellaneous.

OTHER:

CP: Data compilations.

R: Relative values only.

CM: Comments.

F: Forbidden lines.

9. References on lifetimes and transition probabilities

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Ne II: 43
Ne III: 129
Ne VII: 101, 219, 248, 274

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Ni VI: 118
Ni XI: 5
Ni XIV: 246

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WORKING GROUP ON COLLISION PROCESSES

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10. Introduction

Research in atomic and molecular collision processes and spectral line broadening has been very active since our last report (Schultz & Stancil 2005, Allard & Peach 2005). Given the large volume of the published literature and the limited space available, we have attempted to identify work most relevant to astrophysics. Since our report is not comprehensive, additional publications can be found in the databases at the web addresses listed in the final section. Elastic and inelastic collisions among electrons, atoms, ions, and molecules are included and reactive processes are also considered, but except for charge exchange, they receive only sparse coverage.

Numerous meetings on collision processes and line broadening have been held throughout the report period. Important international meetings that provide additional sources of data through their proceedings are: the XXIV International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC) (Fainstein et al. 2006), XXV ICPEAC (Becker et al. 2007), the NASA Laboratory Astrophysics Workshop (Weck et al. 2006), the 18th International Conference on Spectral Line Shapes (ICSLS) (Oks & Pindzola 2006) and the VIth Serbian Conference on Spectral Line Shapes in Astrophysics (SCSLSA)(Popović & Dimitrijević 2007). The 19th ICSLS has just taken place in June 2008.

11. Electron Collisions with Atoms, Ions, Molecules, and Molecular Ions

Collisions of electrons with atoms, ions, molecules, and molecular ions are the major excitation mechanism for a wide range of astrophysical environments. In addition, electron collisions play an important role in ionization and recombination, contribute to cooling and heating of the gas, and may contribute to molecular fragmentation and formation. In the following sections we summarize recent work on electron collisions with astrophysically relevant species, including elastic scattering, excitation, dissociation, ionization, recombination, and electron detachment from negative ions.

11.1. *Electron-Atom Scattering*

New work on elastic scattering from neutral atoms is limited to Xe (Linert et al. 2007), Cs (Zatsarinny & Bartschat 2008), In (Rabasović et al. 2008) and Au (Maslov et al. 2008). The excitation of atomic oxygen has been investigated (Wang & Zhou 2006, Barklem 2007), while new work on ionization has been carried out for Mg (Bolognesi et al. 2008).

11.2. *Electron-Ion Scattering*

For atomic ions, new work has primarily focused on excitation and includes: C^+ (Wilson et al. 2005), N^+ (Hudson & Bell 2005), O^+ (Tayal 2007), Al^{12+} (Aggarwal et al. 2005, Aggarwal et al. 2008), S^{4+} (Hudson & Bell 2006), Ar^{16+} (Aggarwal & Keenan 2005b), Ca^+ (Meléndez et al. 2007), Kr^{6+} (Ishikawa & Vilkas 2008), Fe^+ (Ramsbottom et al. 2007), Fe^{3+} (McLaughlin et al. 2006), Fe^{4+} (Ballance et al. 2007), Fe^{6+} (Witthoeft & Badnell 2008), Fe^{9+} (Aggarwal & Keenan 2005a), Fe^{11+} (Storey et al. 2005), Fe^{15+} (Aggarwal & Keenan 2006), Fe^{17+} (Witthoeft et al. 2006), Fe^{19+} (Witthoeft et al. 2007), Fe^{22+} (Chidichimo et al. 2005), Fe^{25+} (Aggarwal et al. 2008), Ni^{3+} (Meléndez & Bautista 2005), and for Si, Cl, and Ar isonuclear sequences (Colgan et al. 2008).

New elastic data exists for He^+ and Li^{2+} (Bhatia 2008). Ionization and detachment have been studied for H^- (Jung 2008); C^{2+}, N^{3+}, and O^{4+} (Fogle et al. 2008); Ne^{4+} and Au^{47+} (Pindzola et al. 2008); and Si, Cl, and Ar isonuclear sequences (Colgan et al. 2008).

Another important process is recombination for which a number of new works including radiative and dielectronic recombination have appeared: C^{2+}, N^{3+}, and O^{4+} (Fogle et al. 2005); Si^{3+} (Schmidt et al. 2007); Mg^{2+} (Fu et al. 2008); and Fe^{16+} (Chen 2008).

11.3. *Electron-Molecule Scattering*

For molecules, new elastic scattering references have appeared as follows: C_3 (Munjal & Baluga 2006); CH_4 (Cho et al. 2008); H_2CO (Kaur & Baluja 2005); C_6H_6, C_6F_6, C_6H_{12}, C_6H_{14}, C_6F_{14}, C_8H_{16}, C_8H_{18}, and C_8F_{18} (Shi et al. 2008); SF_4 (Szmytkowski et al. 2005); SO_2Cl_2 (Szmytkowski et al. 2006); SiN_2, SiCO, and CSiO (Fujimoto et al. 2007); pyrazine (Winstead 2007); propane (Bettega, da Costa, & Lima 2008); methanol and ethanol (Khakoo et al. 2008); propene and cyclopropane (Makochekanwa et al. 2008); and NeF (Kaur et al. 2008).

For excitation, new references include: H_2 (da Costa et al. 2005, Kato et al. 2008); C_3 (Munjal & Baluga 2006); CH_2 (Allan 2007); CH_4 (Čurik et al. 2008); CO and C_2H_4 (da Costa et al. 2007); CO_2 (Rescigno et al. 2007); CF_4 (Irrera & Gianturco 2005); N_2 (Tashiro & Morokuma 2007, Khakoo et al. 2007), ethene (Allan, Winstead, & McKoy 2008); and NeF (Kaur et al. 2008).

New work for dissociative processes are for dissociative electron attachment to H_2O (Haxton et al. 2007), C_2H_2 (Chourou & Orel 2008, May et al. 2008), and C_4H_2 (May et al. 2008). Research on molecular ionization has been limited to H_2 and D_2 (Martín 2007) and H_2O (Kaiser et al. 2007).

11.4. *Electron-Molecular Ion Scattering*

References on dissociative processes have appeared for: H_2^+ (Motapon et al. 2008), He_2^+ (Buhr et al. 2008), NeH^+ and NeD^+ (Ngassam et al. 2008), H_3^+ (Kokoouline & Greene 2005), D_2H^+ (Zhaunerchyk et al. 2008b), HCO^+ and DCO^+ (Douguet et al. 2008), O_3^+ (Zhaunerchyk et al. 2008a), and $HCNH^+$ (Ngassam et al. 2005).

For excitation, a study has been conducted for H_3^+ (Faure et al. 2006). New results for ionization include H_2^+ (Pindzola et al. 2005), while detachment has been investigated for

Si_2^- (Lindahl et al. 2008). Finally, vibrational excitation due to electron impact has been studied for NeH^+ and NeD^+ (Ngassam et al. 2008).

12. Heavy Particle Collisions

12.1. *Ion-Atom and Atom-Atom Collisions*

Charge exchange has seen a substantial amount of activity over the report period as it plays an important role in a variety of environments. Studies for collisions on H include: H^+ (Bradley et al. 2005, Dubois et al. 2005, Zeng et al. 2008), He^{2+} (Havener et al. 2005), Be^{4+} (Minami et al. 2006), C^{6+} (Liu et al. 2005), N^{2+} and O^{2+} (Barragán et al. 2006a, Barragán et al. 2006c), O^{8+} (Perez & Olson 2005), F^{2+} (Dutta et al. 2005), Ne^{10+} (Errea et al. 2005a, Barragán et al. 2006b), Si^{3+} (Wang et al. 2006, Bruhns et al. 2008), S^{16+} (Janowicz et al. 2005), Cl^{7+} (Zhao et al. 2007), and Ar^{18+} (Errea et al. 2005a). A database for cross sections for all carbon ions colliding with hydrogen has been constructed by Suno & Kato (2006).

Neutral helium is also an important target for which studies have been carried out for the incident ions: He^+ (Bradley et al. 2005), C^{4+} (Hoshino et al. 2007), F^{7+} (Zouros et al. 2008), and $Ne^{(2-6)+}$ (Hasan 2005).

Charge exchange due to proton impact on Ca (Dutta et al. 2006, Pandey & Dubey 2007) and Mg (Pandey & Dubey 2007), alpha particles on Na (Lee 2006), and N^{7+} on atomic oxygen (Perez & Olson 2005) have been studied, while radiative charge transfer in Ne^{2+} collisions with He (Zhao et al. 2006) has been investigated.

Elastic scattering due to proton impact on He, Ne, and Ar (Ovchinnikov et al. 2006) have been studied. Inelastic processes involving hyperfine changing collisions have been investigated for: H + H (Zygelman 2005); $(n-n')$-mixing in $H^*(n) + H(1s)$ collisions (Mihajlov et al. 2005); fine structure transitions for O + H and C + H (Abrahamsson & Krems 2007), $C^+ + H$ and $Si^+ + H$ (Barinovs et al. 2005) and depolarization collisions of excited atoms and ions with hydrogen (Derouich et al. 2005b, Derouich et al. 2005a, Derouich 2007, Derouich & Barklem 2007, Sahal-Bréchot et al. 2007). Electronic transitions have been studied for O + H (Krems et al. 2006) and H impact on S^{3+}, Ar^{13+}, and Fe^{13+} (Burgess & Tully 2005).

Excitation, charge transfer, and ionization due to He^{2+} collisions with H including Debye screening in a dense plasma has been studied by Liu et al. (2008a), Liu et al. (2008b). Electron detachment in He collisions with H^- (Huang et al. 2005, Ogurtsov et al. 2006) and C^- (Huang et al. 2005) has also been investigated. Rate coefficients have been computed for the formation of HD (Dickinson 2005); CH^+ (Barinovs & van Hemert 2005); and SO, SO^+, and S_2 (Andreazza & Marinho 2005) by radiative association.

12.2. *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 He^{2+} (Dubois et al. 2005, Kusakabe et al. 2006), C^{4+} (Zarour et al. 2005), O^+ (Kimura et al. 2006), O^{5+} and Ar^{5+} (Dubois et al. 2005), and F^{7+} (Zouros et al. 2008) with H_2; H^+ (Lindsay et al. 2005a, Wells et al. 2005, Kumar et al. 2006, Lin et al. 2007) and He^{2+} (Kusakabe et al. 2006) with CO; He^{2+} (Abu-Haija et al. 2005b, Kusakabe et al. 2006), $Ar^{5,4+}$ (Abu-Haija et al. 2005a), and Kr^{8+} (Kaneyasu et al. 2005) with N_2; H^+ and O^+ (Luna et al. 2005), He^{2+} (Abu-Haija et al. 2005b, Kusakabe et al. 2006), and $Ar^{5,4+}$ (Abu-Haija et al. 2005a) with O_2; H^+ (Kimura et al. 2006), He^{2+} (Bodewits, et al. 2005, Seredyuk et al. 2005c), O^{6+} (Seredyuk et al. 2005b, Bodewits & Hoekstra 2007), and a range of ions (Otranto & Olson 2008) with water; H^+ (Lindsay et al. 2005a), He^{2+} (Abu-Haija et al. 2005b, Kusakabe et al. 2006), and O^{6+} (Seredyuk et al. 2005b) with CO_2; H^+ with NH_2 (Suno et al. 2006); He^{2+} (Abu-Haija et al. 2005b, Kusakabe et al. 2006) with NH_3; H^+ (Lindsay et al. 2005b), He^{2+} (Seredyuk et al. 2005a), and C^{4+} and O^{6+} (Seredyuk et al. 2005b) with CH_4; H^+ (Suzuki et al. 2005) and He^{2+} (Seredyuk et al. 2005a) with C_2H_4; and He^{2+} (Seredyuk et al. 2005a) with C_2H_6. Other charge exchange studies include H_2^+ + H (Errea et al. 2005b); $N_2^+ + N_2$ and $O_2^+ + O_2$ (Tong & Nanbu 2007); and $O^+ + O_2$ (Martinez et al. 2006), while Cornelius (2006) has developed a scaling relation for total cross sections with H_2.

For applications to x-ray emission from comets and planetary atmospheres, charge exchange has been considered for molecular targets including $C^{(3-6)+}$, $N^{(4-7)+}$, and $O^{(5-7)+}$ with methane (Djurić et al. 2008); highly charged L-shell Fe ions with various neutrals (Wargelin et al. 2005, Beiersdorfer et al. 2008); and for a range of ions and molecules (Otranto et al. 2006).

The internal level populations of molecular rovibrational states are primarily controlled through collisional excitation by atom and molecule impact. Investigations have been carried out for excitation of H_2 by H (Wrathmall & Flower 2006, Wrathmall et al. 2007), He (Mack et al. 2006), H_2 (Lee et al. 2006), and H^- (Giri & Sathyamurthy 2006); HF by He (Reese et al. 2005); CO by H (Yang et al. 2006a, Shepler et al. 2007), He (Yang et al. 2006a), and H_2 (Wernli et al. 2006, Yang et al. 2006b); CO^+ by H (Andersson et al. 2008); CN by C_2H_2 (Olkhov & Smith 2007); CS by He (Lique et al. 2006b, Lique & Spielfiedel 2007); PN by He (Tobola et al. 2007); SiO by H (Palov et al. 2006) and He (Dayou & Balança 2006); SiS by He (Vincent et al. 2007); SO by He (Lique et al. 2006a, Lique et al. 2006c); H_2O by He (Yang & Stancil 2007) and H_2 (Dubernet et al. 2006), NH_3 (Machin & Roueff 2005, Yang & Stancil 2008), NH_2D (Machin & Roueff 2006), and ND_2H by He (Machin & Roueff 2007); and HC_2N by He and H_2 (Wernli et al. 2007).

Other investigations include: collisional dissociation of highly excited H_2 by He Ohlinger et al. (2007), fragmentation of CO by slow C^{6+} and Ar^{11+} (Wells et al. 2008), and dissociation and fragmentation of N_2 by slow Xe^{q+} ions, (q=15-21), (Zhu et al. 2005). Mutual neutralization in H_2^+ collisions with H^- has been studied by Liu et al.(2006) and the formation of HeH_2^+ via radiative association by Mrugala & Kraemer (2005).

13. Reactive Scattering and Chemistry

Due to space limitations, we cannot review the many advances in reactive scattering and chemical processes relevant to astrophysics. One noteworthy and relevant study involves a quasiclassical trajectory investigation of $H + CH_4 \rightarrow H_2 + CH_3$ (Xie et al. 2006), and updates to the UMIST Astrochemistry database which gives rate coefficient fits for 4572 reactions, has been completed recently (Woodall et al. 2007).

14. Stark broadening

Knowledge of line widths and shifts for atomic transitions is very important for the interpretation of stellar spectra and also for circumstellar conditions and galactic H II regions.

The Critical Review of Selected Data on Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms for the period 2001-2007, see Lesage (2008), contains tables where measured values are listed and compared with semi-classical calculations. A book entitled 'Stark Broadening of Hydrogen and Hydrogenlike Spectral Lines in Plasmas' has been published by Oks (2006) and contains many useful references.

14.1. *Developments in line broadening theory*

Poquérusse & Alexiou (2006) have extended standard semi-classical impact theory for hydrogen-like ions to include penetrating collisions. For transitions in highly excited hydrogen-like atoms and ions Stambulchik & Maron (2008) have produced a simple analytical method for calculating line shapes and Gigosos et al. (2007) have developed an exact expression for the impact broadening operator of hydrogen. The asymmetry of hydrogen lines has been studied by Demura et al. (2008a) and Demura et al. (2008b).

Stambulchik & Maron (2008) have studied broadening of lines subject to external electric and magnetic fields and Godbert-Mouret et al. (2006) have developed new code to calculate their lineshapes. Dubau et al. (2007) have carried out quantum mechanical calculations of electron impact broadening for XUV lines in plasmas.

14.2. *Isolated lines*

For isolated lines, Stark broadening is dominated by collisions with plasma electrons. Broadening parameters have been determined theoretically for:

Ar II 476.5 nm, 480.6 nm and Kr II 469.4 nm lines (Dimitrijević & Csillag 2006), Cd I 33 singlets and 37 triplets (Simić et al. 2005a), 26 Ne V multiplets (Hamdi et al. 2007) and 15 Si VI multiplets (Hamdi et al. 2008).

Also for: 4 N IV, 3 O V, 1 F VI and 4 Ne IV (Elabidi et al. 2008a), 2 N II, O III, F IV and Ne V (Ivković et al. 2005), O II (Mahmoudi et al. (2005)), F II (Srećković et al. 2005b), 1 F III (Simić et al. 2005b), 6 Ar I (Dimitrijević et al. 2007a), 9 Cr I (Dimitrijević et al. 2005), 3 Mn II (Popović et al. 2008), 3 Te I (Dimitrijević et al. 2007b, Dimitrijević et al. 2008), F III (Simić et al. 2005b), Ne VII, Ne VIII and Si XI (Elabidi et al. 2008b), S II, S III and S IV (Milovanović N. & Dimitrijević 2007), Cu III, Zn III and Se III (Simić et al. 2006), Ga II (N'Dollo & Donga-Passi 2006), Sn II (Colón & Alonso-Medina 2006) and Pb III (Alonso-Medina et al. 2008) lines.

Broadening parameters have been obtained experimentally for:

C I 247.8561 nm (Djeniže et al. 2006b), Mg II 448.1 nm (Djeniže et al. 2005b), Fe I 381.58 nm (Bengoechea et al. 2006) and Fe I 538.34 nm (Bengoechea et al. 2005) lines.

Also for: 2 N I (Bartecka et al. 2005), 3 O II (Bukvić et al. 2005), 23 O III (Srećković et al. 2005a), 10 N II and 8 O III (Ivković et al. 2005), F II (Srećković et al. 2005b), 4 Ne I (Dzierżega et al. 2006), 13 Ne I (Jovićević et al. 2005), 7 Ar I (Milosavljević et al. 2006), 6 Ar II (Iglesias et al. 2006), 6 Mn I (Srećković et al. 2007), 11 Mn II and 3 Mn III (Djeniže et al. 2006e), 17 Ni II (Mayo et al. 2008), 35 Kr II (del Val et al. 2008), 2 Ag I and 2 Au I (Djeniže et al. 2006c), 2 Ag I, 11 Ag II and 3 Ag III (Djeniže et al. 2005a), 26 Au II (Ortiz & Mayo 2005), 43 Sn I and 27 Sn II (Alonso-Medina & Colón 2008), 12 Sn I and 16 Sn II (Djeniže et al. 2006d), 16 In III (Djeniže et al. 2006a), 10 Pb III lines (Alonso-Medina & Colón 2007), 31 Pb II (Colón & Alonso-Medina 2006), 38 Xe III (Peláez et al. 2006a) and shifts of 110 Xe and 42 Xe III (Ćirišan et al. 2006) lines.

Djurović et al. (2006) have presented a review of experimental work on Stark broadening of 80 singly ionized xenon lines and Purić et al. (2008) have used published Stark widths for spectral lines originating from 3s-3p transition arrays of multiply charged ions, to establish trends from which Stark widths are predicted for Mg VII, Mg IX, Mg X, Na VII, Na VIII, Al VIII, Al IX, Si XI, Ti XI, Cr XIII, Cr XIV, Fe XV, Fe XVI, Fe XXIII and Ni XVIII.

Stehlé et al. (2005) have examined current Stark broadening theory as a basis for diagnostics of low-temperature plasmas and Mahmoudi et al. (2008) have provided new expressions for diagonal multiplet factors of complex configurations, required for studies of isolated lines. Zmerli et al. (2008) have proposed an improved interpolation method for widths as a function of temperature.

14.3. *Transitions in hydrogenic and helium-like systems*

New quantum mechanical calculations of the broadening of Lyβ, Lyγ and Lyδ have been carried out by de Kertanguy et al. (2005). Transitions in the Balmer series have been studied by Gigosos & González (2006), and by Stambulchik et al. (2007) for $n \leqslant 15$. Broadening of high-n transitions are considered by Lisgo et al. (2006) and benchmarked against electron density measurements. New experiments for Hβ for the wide range of plasma parameters have been carried out by Djurović et al. (2005) and Griem et al. (2005) compare Hα profiles measured at high electron densities with theoretical results.

Broadening of the radio recombination lines of hydrogen has been studied theoretically by Watson (2006) and Gavrilenko & Oks (2007) and lines of hydrogen-like and helium-like ions of C, Si and Ar have been examined by Stambulchik & Maron (2006) who find that ion dynamics is very important.

New theoretical calculations of broadening have been reported for He I 667.8 nm and 587.6 nm lines (Ben Chaouacha et al. (2007)) and He I 728.1, 706.5, 504.8, 492.2 and 471.3 nm lines in a dense plasma (Omar et al. (2006)). Peláez et al. (2006b) have carried out experiments for He I 318.8 nm and 402.6186 nm lines.

15. Broadening by neutral atoms and molecules

The analysis of experimental molecular spectra in order to extract line shape parameters is often very difficult. Line shapes can be affected by collisional narrowing and the dependence of collisional broadening and shifting on molecular speed. When these effects are sufficiently important, fitting Voigt profiles to experimental spectra produces systematic errors in the parameters retrieved.

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).

15.1. *Broadening of atomic lines*

Some theoretical work has been published in the period 2005-2008 and the transitions with the perturbing atoms or molecules are listed below.

Li; 2s-3s transition broadened by Ar, Kr and Xe (Rosenberry et al. 2007).
Li; wings of the resonance line broadened by He and H_2 (Allard et al. 2005).
Na and K; wings of the resonance lines broadened by He (Zhu et al. 2006).
Li, Na and K; impact widths for the resonance lines broadened by He (Mullamphy et al. 2007).
Rb and Cs; resonance line profiles, including far line wings, broadened by He and H_2 (Allard & Spiegelman 2006).
Fe II; 24188 lines broadened by collisions with H (Barklem & Aspelund-Johansson 2005).
Sr: $5s^2\,{}^1S_0 \rightarrow 5s5p\,{}^3P_1$ and $5s5p\,{}^3P_{0,1,2} \rightarrow 5s6s\,{}^3S_1$ transitions broadened by the rare gases (Holtgrave & Wolf 2005).

15.2. *Broadening and shift of molecular lines*

Much new data have been published since the last report was prepared. The molecules are listed below with their perturbing atomic or molecular species and are labelled by 'E' and 'T' to indicate experimental work and theoretical analysis respectively.

H_2-H_2 collision-induced absorption (T) (Orton et al. 2007); in binary mixtures H_2-N_2 and H_2-CO (E) (Abu-Kharma et al. 2006).
H_2 lines broadened and shifted by He (T) (Ma et al. 2007).
HDO lines broadened and shifted by N_2 (E) (Bach et al. 2005).
HCN lines broadened and shifted by HCN and air (E) (Devi et al. 2005); N_2 (E) (Smith et al. 2008); H_2, N_2, O_2, CH_3CN and rare gases (E) (Rohart et al. 2007).
HC_3N lines broadened by H_2, He and N_2 (E) (Colmont et al. 2007b).
H_2CO lines broadened by H_2CO, N_2 and O_2 (E) (Staak et al. 2005).
HCO^+ lines broadened by He and Ar (T) (Buffa 2007).
HNO_3 lines broadened by air (E) (Cazzoli et al. 2005).
HO_2 lines broadened by air (E) (Ibrahim et al. 2007); H_2O and N_2 (E) (Kanno et al. 2005).
HI lines broadened by HI (E) (Bulanin et al. 2005, Hartmann et al. 2005); He (E) (Flaud et al. 2006).
HI, HBr lines broadened by rare gases (E) (Domanskaya et al. 2007).

H_2O lines broadened by H_2O (T) (Tolchenov & Tennyson 2005, Ptashnik et al. 2005, Antony & Gamache 2007, Antony et al. 2007); air (E) (Liu et al. 2007, Seta et al. 2008); H_2O and air (E+T) (Toth 2005, Jenouvrier et al. 2007, Ibrahim et al. 2008); N_2 (E+T) (Aldener et al. 2005, Bandyopadhyay et al. 2007, Tran et al. 2007, Bykov et al. 2008); N_2 and air (E+T) (Aldener et al. 2005, Bandyopadhyay et al. 2007, Tran et al. 2007, Bykov et al. 2008, Hodges et al. 2008); N_2 and O_2 (E) (Golubiatnikov et al. 2008, Hoshina et al. 2008); H_2O, N_2 and O_2 (E) (Cazzoli et al. 2007, Koshelev et al. 2007, Cazzoli et al. 2008); H_2O and Ar (E) (Li et al. 2008); H_2O, H_2, N_2, O_2, CO_2 and rare gases (E) (Golubiatnikov 2005); H_2O, H_2, N_2, O_2, CO_2, He and air (E) (Brown et al. 2005).

CH_4 lines broadened by air (E) (Predoi-Cross et al. 2006); CH_4 and air (E) (Predoi-Cross et al. 2007a); CH_4, air, He and H_2 (E) (Lucchesini & Gozzini 2007); CH4 (E) (Lepère 2006, Wishnow et al. 2007); H_2 and He (T) (Tran et al. 2006); N_2 (E) (Mondelain et al. 2007, Martin & Lepère 2008); CH_4 and N_2 (E) (Menard-Bourcin et al. 2007); N_2 and O_2 (E) (Mondelain et al. 2005, Lepère et al. 2005); N_2, O_2 and air (T) (Antony et al. 2008).
C_2H_2 self-broadened lines (E+T) (Lepère et al. 2007, Nguyen et al. 2008, Lyulin et al. 2008); broadened by He (T) (Thibault 2005, Nguyen et al. 2006); H_2, D_2, N_2, air and rare gases (E) (Arteaga et al. 2007); CO_2 (E+T) (Martin et al. 2006).
C_2H_4 lines broadened by N_2 (E) (Blanquet et al. 2005).
C_3H_2 lines self broadened (E) (Achkasova et al. 2006).
CH_3Br lines broadened by N_2 (E+T) (Jacquemart et al. 2007, Tran et al. 2008); CH_3Br and N_2 (E) (Jacquemart & Tran 2008).
CH_3F lines broadened by H_2 (E) (Lerot et al. 2006b); N_2, O_2 (E) (Lerot et al. 2006a); CH_3F (Lerot et al. 2005).
CH_3CN broadened by CH_3CN and N_2 (E) (Rinsland et al. 2008).

CO lines broadened by He (E) (Thibault et al. 2007); CO_2 (E) (Sung & Varanasi 2005); Ar (E+T) (Wehr et al. 2006a, Wehr et al. 2006b); N_2, O_2, CO_2 and rare gases (Colmont et al. 2007a).
CO_2 lines broadened by air (E) (Predoi-Cross et al. 2007c, Toth et al. 2007); self-broadened lines (E) (Hikida et al. 2005, Le Barbu et al. 2006, Predoi-Cross et al. 2007b),

(T) (Toth et al. 2006); air and CO_2 (E) (Devi et al. 2007a, Toth et al. 2008, Joly et al. 2008, Devi et al. 2007a); air and Ar (E) (Li et al. 2008); N_2 and O_2 (E) (Hikida & Yamada 2006).
Cs_2 lines broadened by N_2 (E+T) (Misago et al. 2006); O_2 (E+T) (Misago et al. 2007); Ar and air (E+T) (Misago et al. 2008).

N_2 self-broadened lines (E) (El-Kader & Moustafa 2005, Hashimoto & Kanamori 2006); N_2-H_2 collision-induced absorption (E) (Boissoles et al. 2005).
NH_3 lines broadened by NH_3 (E) (Leary et al. 2008); N_2, O_2 and air (Dhib et al. 2007).
N_2O lines broadened by air (E) (Grossel et al. 2008).

O_2 self-broadened lines (E) (Tretyakov et al. 2007, Predoi-Cross et al. 2008a); lines broadened by O_2 and N_2 (Tretyakov et al. 2005); N_2 (E+T) (Predoi-Cross et al. 2008b).
O_3 lines broadened by O_3 (E) (Yamada & Amano 2005); N_2 and O_2 (E+T) (Rohart et al. 2008).
OCS lines broadened by OCS (E) (Matton et al. 2006); N_2 and O_2 (E) (Koshelev et al. 2006).
PH_3 lines broadened by N_2 (E+T) (Bouanich et al. 2005, Bouanich & Blanquet 2007).
SO_2 self-broadened lines (E+T) (Zéninari et al.. 2007, Henningsen et al. 2008).

16. Databases

A database for atomic and molecular processes is maintained at the Oak Ridge National Laboratory Controlled Fusion Atomic Data Center (CFADC) at the address:

http://cfadc.phy.ornl.gov

and a useful online database of rovibrational collisional excitation data, BASECOL, can be found at:

http://basecol.obspm.fr .

Some collisional data are also available on the Leiden Atomic and Molecular Database:

http://www.strw.leidenuniv.nl/˜ moldata

and the UMIST Astrochemistry database is at:

http://www.udfa.net .

A 'virtual observatory' for astronomers can be found at:

http://cdsarc.u-strasbg.fr

and the latest version of the database High resolution Transmission, HITRAN 2004, is 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) has address:

http://icb.u-bourgogne.fr/OMR/SMA/SHTDS/STDS .

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 2008 and the database at the Observatoire de Paris,

http://amrel.obspm.fr/balss

contains a Bibliography up to 2007. The Vienna Atomic Line Database (VALD) can be found at:

http://ams.astro.univie.ac.at/˜ vald

and the Belgrade database at:

http://www.aob.bg.ac.yu/BELDATA .

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WORKING GROUP ON SOLIDS AND THEIR SURFACES

CHAIR **Gianfranco Vidali**

SEXENNIAL REPORT 2003-2009

17. Introduction

In the last decade there has been a tremendous increase of interest in studying processes occurring on interstellar dust. In part this is due to the availability of ground-based and space-borne high quality instruments which have been used to detect molecules in diverse astrophysical environments, from protoplanetary disks to hot cores and dense clouds. It has also been recognized that interstellar dust has an important role in the formation of molecules, from molecular hydrogen to methanol. Therefore, it is necessary not to study only properties of dust, but also understand how atoms and molecules interact with and on dust.

This has prompted a number of laboratories with a tradition of working in surface science to study the processes associated with dust. Besides the standard probes that have been used in the past, now there are available techniques that can give precise information at the atomic/molecular level about the formation of molecules on dust. For instance, Thermal Programmed Desorption (TPD), Reflection Absorption Infrared Spectrometry (RAIRS), Resonant Enhanced Multiphoton Ionization (REMPI), and Atom Force Microscopy (AFM) give information about the kinetics and energetics of diffusion of atoms/molecules on and desorption from surfaces, the products of reaction, the ro-vibrational state of ejected products, and the morphology of the solid surfaces, respectively. One of the consequences of the interest by surface science laboratories in studying physical/chemical properties of dust analogues and reactions occurring on them is that works of interest to astrochemistry are now regularly published in chemical physics/ surface science journals such as J. Chem. Phys., J. Phys. Chem., Phys. Chem. Chem. Phys., Surface Science, and others.

While in the past there has been a large number of laboratory studies of the interaction of charged particles and radiation with ice-covered dust grain analogues, most recent work points at new directions of research that will likely continue to be studied in the near future, i.e. the formation of molecules in/on ices by hydrogenation reactions, the properties of mixed ices, and the formation and properties of dust particles, including nanoparticles. Observations with ALMA, SOFIA and HERSCHEL will yield more detailed information on dust and molecules, and theoretical studies will need to sort out the role of dust particles in molecule formation.

Meetings

Sessions about atomic/molecular interaction with surfaces are often featured at regularly scheduled COSPAR, AAS and Lunar and Planetary Institute meetings. For more information about these meetings, visit the Web sites of the respective organizations. For information about the meetings below, go to the Web site of the Canadian Astronomy Data Centre (Web link: http://www1.cadc-ccda.hia-iha.nrc-cnrc.gc.ca/meetings/). Unfortunately, a number of meetings' official Web sites have been taken down.

Most important meetings (listed in inverse chronological order):

- Cosmic Dust - Near And Far, Heidelberg Convention Center Heidelberg, Germany. 9/8/08-9/12/08
- Bridging the Laboratory and Astrophysics, a Meetin-in-a-Meeting, AAS 212th, St. Louis, MO, 6/1/08-6/5/08
- The Molecular Universe: An International Meeting on the Physics and Chemistry of the Interstellar Medium, Arcachon, France 5/5/08-5/8/08
- AbSciCon 2008: The Fifth Astrobiology Science Conference, Santa Clara, CA 4/15/08-4/17/08
- Second Workshop : Titan Observations, Experiments, Computations, and Modeling, Miami, FL 3/24/08-3/26/08
- IAU Symposium No. 251: Organic Matter in Space, Hong Kong 2/18/08-2/22/08
- The Evolving Insterstellar Medium in the Milky Way and Nearby Galaxies, Pasadena, CA 12/2/07-12/5/07
- Bioastronomy 2007: Molecules, Microbes, and Extraterrestrial Life San Juan, PR 7/16/07-7/20/07
- 2007 Gordon Conference on Origins of Solar Systems, Mount Holyoke College, South Hadley, MA 7/8/07-7/13/07
- Molecules in Space and Laboratory, Paris, France 5/14/07-5/18/07
- Les Houches Winter School: Astronomy in the Submillimeter and Far Infrared Domains with the Herschel Space Observatory, Les Houches, France 4/23/07-5/4/07
- Titan Observations, Experiments, Computations, and Modeling, Honolulu, HI 2/5/07-2/7/07
- Science with ALMA: a New Era for Astrophysics, Madrid, Spain 11/13/06-11/16/06
- Heidelberg Summer School on the Interstellar Medium, Heidelberg, Germany 9/25/06-9/29/06
- From Dust to Planetesimals, Ringberg Castle, Bavaria, Germany 9/11/06-9/15/06
- Nobel Symposium on Cosmic Chemistry and Molecular Astrophysics, Sudertuna, Sweden 6/10/06-6/15/06
- Complex Molecules in Space; present Status and Prospects with ALMA, Fuglsocentret, Denmark 6/8/06-6/11/06
- Carbon in Space, International workshop, Villa Vigoni, Lago di Como, Italy, 6/22/06-6/25/06
- NASA Laboratory Astrophysics Workshop, Las Vegas, NV 2/14/06-2/16/06

- Astrochemistry - A Molecular Approach [Symposium 47; Pacifichem 2005), Honolulu, HI 12/18/05-12/17/05
- Hunt for Molecules, Paris, France 9/19/05-9/20/05
- Protostars and Planets V, Hawai'i Island, HI 10/24/05-10/28/05
- 5th. European Workshop on Astrobiology, Budapest, Hungary 10/10/05-10/12/05
- IAU Symposium No. 231: Astrochemistry throughout the Universe: Recent Successes and Current Challenges, Monterey, CA 8/29/05-9/2/05
- Astrobiology and the Origins of LIfe, McMaster University, Hamilton, Canada 5/24/05-6/10/05
- The Spitzer Space Telescope: New Views of the Cosmos, Pasadena, CA 11/9/04-11/12/04
- The Dusty and Molecular Universe:A prelude to HERSCHEL and ALMA, Paris, France 10/27/04-10/29/04
- AOGS 2004 Session SP2: Effects of Space Radiation on Solar System Ices, Singapore 7/5/04-7/9/04
- Astrophysics of Dust, Estes Park, CO , 2003

Published works in the area of molecular reactions on solid surfaces have been sorted in 4 sections:

(*a*) Reviews
(*b*) Observations of dust and ices in the ISM
(*c*) Dust (formation, properties, and exposure to space environment)
(*d*) Interactions of atoms and molecules with solids in simulated ISM conditions
(*e*) Interaction of radiation and charged particles with ices in simulated ISM conditions

Obviously, there is a certain degree of arbitrariness in the sorting. Several papers could be entered in more than one section. The papers listed here are the ones that appeared in print since the last review by the Working Group on Molecular Reactions on Solid Surfaces in 2002; therefore, this report covers a six-year period. Works are listed in inverse chronological order.

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