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COMMISSION 14: ATOMIC AND MOLECULAR DATA[1]

(DONNEES ATOMIQUES ET MOLECULAIRES)

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

This report is one of the main contributions of Commission 14 to the astronomical community. It comprises six Sections prepared by the Working Groups of Commission 14. It is also available on the Commission 14 Website:
http://cfa-www.harvard.edu/amdata/IAU_14.

1. ATOMIC SPECTRA AND WAVELENGTH STANDARDS
2. ATOMIC TRANSITION PROBABILITIES
3. COLLISION PROCESSES
4. LINE BROADENING
5. MOLECULAR STRUCTURE AND TRANSITION DATA
6. MOLECULAR REACTIONS ON SOLID SURFACES

In addition to this report, one Joint Discussion at the XXVth IAU General Assembly was organized by this Commission and the Commission is participating in two more:

JD 17 ATOMIC DATA FOR X-RAY ASTRONOMY (organized);
JD 20 FRONTIERS OF HIGH RESOLUTION SPECTROSCOPY;
JD 21 THE ASTROCHEMISTRY OF EXTERNAL GALAXIES.

[1] Commission of the Executive Committee.

1. WORKING GROUP ON ATOMIC SPECTRA AND WAVELENGTH STANDARDS

(GROUPE DE TRAVAIL POUR LES SPECTRES ET LONGUEURS D'ONDE ATOMIQUES)

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.

Be II (J1), **Be III** (J2), **C IV** (G1), **Ne IV** (K6), **Ne V** (K7), **Ne VI** (K8), **Al I** (B2), **Al II, III** (G1), **Si II, IV** (G1), **S VII** (J3), **Ar I** (W2), **Cr II** (P3), **Fe V** (A1), **Ni II** (P3), **Zn I, Zn II** (G2, P3), **Ga I, Ga II** (K3), **Nb II** (R1), **Mo II** (N2), **Tc I** (P1), **Ru II**(K5), **Pd II** (L2), **Ag I** (P2), **Ag II** (K1), **In I, In II** (K4), **Sb III** (T1), **Ba I,II** (K2), **Pr II, Pr III** (I1), **Tb II** (L1), **Dy I, II** (N1), **Yb III** (B1), **Ta II** (E2), **W II** (E1), **Os I** (K9), **Hg II** (S1), **Bi I, II, III** (W1)

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. For details about spectra of rare earth elements, see Wahlgren (2002). The data in a number of the references above include and/or supersede all or most of the previously available energy-level and/or wavelength data for the indicated spectrum.

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). There is a renewed interest for spectral data of rare earth elements in lighting industry and astrophysics, which reflects the activities at most laboratories.

1.2. Wavelength Standards

An atlas of a thorium-argon hollow cathode lamp in the 1-2.5 μm region has been published by Hinkle et al. (2001) to be used for calibration of near-infrared spectra. A new campaign for very accurate wavelengths of selected lines has been initiated by the current work on the time variability of the fine structure constant (Webb et al. 2001). For this purpose two papers on accurate wavelengths measurements of selected lines in Cr II, Ni II and Zn II performed at Lund and London (P3) and on CIV, Si IV, AlIII, Al II, Si II at NIST (G1) have been published during the last 3 years. The data will also be applicable to spectroscopy of the interstellar medium.

1.3. Larger Compilations, Reviews, Conference Proceedings

We will mention a few compilations that have appeared during the period 1999-2002, as most data are now available in various databases via Internet; some databases are listed in the next section. Shirai et al. (2000) have published a compilation on *Highly Ionized Atoms* (Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, Mo). New compilations on spectra of neon at various ionization stages are included in the list of elements above. Morton (2000) has pubslihed a compilation of *Atomic Data for Resonance Absorption Lines. II. Wavelengths*

Longward of the Lyman Limit for Heavy Elements. A third compilation in this series is to be submitted by Morton. A new *Handbook of Basic Atomic Spectroscopic Data* has been compiled by Sansonetti and Martin (2002) at NIST and it will be a very useful tool for stellar spectroscopy. It contains fundamental spectral lines of all elements (H-Es) in the lowest ionization stages. A coming compilation of spectral data for the Chandra X-ray Observatory is also announced by NIST. Both these will be available as databases (see below).

A number of papers on atomic spectroscopic data are included in proceedings of the *Seventh International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, held in Belfast, UK, August 2001. Invited papers are published in Physica Scripta's T Series (Hibbert & Wiese 2002), and especially the paper by Wahlgren (2002) gives a comprehensive review of the current spectroscopic status for the rare earth elements. Abstracts of the contributed papers were distributed at the meeting. A few papers on astrophysical data needs are included in the proceedings from the second and third international conference *ICAMDATA*, held at Oxford, UK, in March 2000 and in Gatlinburg, USA, April 2002. Several papers deal with atomic databases. Proceedings from the EGAS (European Group of Atomic Spectroscopy) conferences appear in the Physica Scripta T-series: 31^{st} EGAS T86 (2000) and 32^{nd} EGAS T95 (2001).

1.4. Atomic Spectroscopic Data on the Internet

The URL addresses for a number of World Wide Web sites offering laboratory data of the types covered by Working Groups 1 and 2 are listed below. The italicized names of particular databases or datasets are followed by symbols CL, EL, TP in parentheses, indicating types of data:

CL Experimental wavelengths given with energy-level classifications;
EL Experimental values for energy levels;
TP Transition probabilities and/or related quantities (oscillator strengths etc.).

A Weizmann Institute site maintains an updated list of atomic databases and datasets on the Internet: *Databases for Atomic and Plasma Physics* (Weizmann Inst. of Science, Israel)

http://plasma-gate.weizmann.ac.il/DbfAPP.html

This site has links to most of the databases listed here as well as to a number of others. Instructions are given for e-mail access to data from the *Vienna Atomic Line Data-Base* (CL, TP) and for ftp downloading of a *Spectral Bibliography Database (BIBL)*, developed and maintained by the Institute of Spectroscopy, Russia.

The *NIST Atomic Spectra Database* version 2.0, released in March 1999, includes data (CL, EL, TP) that have been critically compiled either at NIST or by other reliable sources. The version 2.1 is coming soon. The new Handbook at NIST will also be available as a database as well as the spectral data for the Chandra X-ray observatory.

http://physics.nist.gov/asd

The database contains CL, EL, and TP for H-Ni (Z=1-28), with additional EL for H-Kr (Z=1-36), Mo (Z=42) and the lanthanides (Z=57-71). The prominent lines from the first five ionization stages are included for Cu to Es (Z=29-99). The database also contains a compilation of "Ground Levels and Ionization Energies for the Neutral Atoms".

Spectral information can be obtained at *CDS* (Centre de Données Astronomiques de Strasbourg, France) and the *ADC, Astronomical Data Center* at NASA Goddard Space Flight Center, U.S.A.

http://cdsweb.u-strasbg.fr/cats/VI.htx
http://adc.gsfc.nasa.gov/adc/sciencedata.html.

At CDS choose from a list of catalogues including several with extensive atomic spectroscopic data, and use the search facility at ADC to get data on CL, EL, and TP.

The *AMODS* (The Atomic Molecular and Optical Database System) database at Korea Atomic Energy Research Institute contains atomic data (EL,CL,TP) from the CDS and

NIST databases on a menu at
http://amods.kaeri.re.kr.

By selecting "Databases" at *CfA Atomic $ Molecular Physics Division* (Harvard-Smithsonian Center for Astrophysics),
http://cfa-www.harvard.edu/amp,
one gets access to the widely used data on *Kurucz CD-ROM 18* and *Kurucz CD-ROM 23* (CL, TP) and the UV/VUV line list (CL) of Kelly.. There are also links to other sites. The Kurucz data can also be found on the European server at
http://www.pmp.uni-hannover.de/projekte/kurucz/sekur.html.

Theoretical data (EL,TP) on selected ions of the elements, Cr, Mn, Fe, Co and Ni are available via ftp from "Atomic Physics Theory" at the University of Amsterdam:
ftp://ftp.wins.uva.nl/pub/orth.

The compilation of "Atomic Data for Resonance Absorption Lines" at Herzberg Institute of Astrophysics, Canada, is located at
http://www.hia.nrc.ca/STAFF/dcm/atomic_data.html.

The *Atomic Data for Astrophysics* (University of Kentucky, U.S.A.) has a database on "Energy Levels, Wavelengths, Transition Probabilities" (CL, TP) and a number of links to other databases and datasets.
http://www.pa.uky.edu/~verner/atom.html.

A new database for rare earth spectra has been installed at Mons University in Belgium
http://www.umh.ac.be/~astro/dream.shtml.

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K3 Karlsson, H., & Litzén, U. 2001, J.Phys B:At.Mol.Opt.Phys 33, 2929

K4 Karlsson, H., & Litzén, U. 2001, J.Phys B:At.Mol.Opt.Phys 34, 4475

K5 Karlsson, H., Joueizadeh, A.,& Johansson, S. 2002, Phys. Scr. 63, 238

K6 Kramida, A.E., *et al.* 1999, Eur.Phys.J. D7, 525

K7 Kramida, A.E., *et al.* 1999, Eur.Phys.J. D7, 547

K8 Kramida, A.E., *et al.* 1999, J.Opt.Soc.Am. B16, 1966

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P3 Pickering, J.C., *et al.*, 2000, MNRAS319, 163
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Shirai, T., *et al.* 2000, J.Phys. Chem. Ref. Data, Monograph 8
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2. WORKING GROUP ON ATOMIC TRANSITION PROBABILITIES
(GROUPE DE TRAVAIL POUR PROBABILITES DE TRANSITION ATOMIQUES)

CHAIR: W.L. Wiese
CO-CHAIR: J.R. Fuhr

The Atomic Spectroscopic Data Center at the National Institute of Standards and Technology (NIST) Gaithersburg, MD 20899, USA is continuing its critical data compilation and bibliographical work. It has contributed all its evaluated transition probability material to a greatly expanded version 2.0 of the NIST atomic spectroscopic database, which is on the World Wide Web. This database contains about 50,000 transition probabilities with estimated uncertainties and may be accessed via links from the NIST Physics Laboratory WWW homepage at http://physics.nist.gov/.

A comprehensive NIST bibliographical database on atomic transition probabilities, which now contains approximately 7500 entries, has been updated through July 2002, and is also available at the above-cited World Wide Web site. The current compilation work on atomic transition probabilities at NIST is centered on the evaluation and tabulation of numerical data for the lighter elements and on Fe I and Fe II. Work is in progress on hydrogen, helium, lithium, beryllium, boron, sodium, magnesium, aluminum, silicon, and sulfur. The tabulations include allowed (electric dipole) as well as forbidden (mainly magnetic dipole and electric quadrupole) lines.

The following major tabulations of transition probability data were published during the latest 3-year period:

(a) The MCHF/MCDHF Collection was recently established and put on the Web by C. Froese Fischer et al. [79]. It contains a large number of transitions for Li-like through Al-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.

(b) The D.R.E.A.M. database (Database on Rare Earths at Mons University) [17] contains wavelengths, energy levels, oscillator strengths and radiative lifetimes

for neutral, singly and multiply-ionized rare earth elements with atomic numbers $57 \leq Z \leq 71$. Presently, it contains about 55,000 lines for 23 ions, mostly for singly and doubly charged species, and further extensions are planned for the near future. It is also available on the Web.

(c) Atomic spectral tables for numerous ions of Ne, Mg, Si, and S in the 10–170 Å region have been compiled by Podobedova et al. [145] These tables, containing about 3200 lines, were specifically prepared for X-ray space observatories, such as Chandra.

(d) The NIST data center recently published a 632-page volume of spectral data for highly ionized atoms of Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr and Mo as Monograph 8 of the Journal of Physical and Chemical Reference Data [161]. This volume contains atomic transition probabilities for a substantial fraction of the 16,000 spectral lines tabulated in this book. It is planned to put these data on the Web.

(e) Transition probabilities for the resonance lines of heavier elements have been compiled by Morton [123]. He has tabulated about 150 lines of the elements Ge ($Z = 32$) through Bi ($Z = 83$) plus some data for Tc, Th and U.

(f) The fourth edition of Allen's widely used Astrophysical Quantities handbook [51] contains a chapter on "Spectra" by Cowley et al., which lists 270 oscillator strengths for prominent lines of numerous astrophysically important spectra and approximately 160 A-values for magnetic dipole and electric quadrupole (forbidden) transitions.

(g) A few other atomic databases have recently been established that contain transition probability data but are of a more general nature. The emphasis, e.g., for the CHIANTI [102] and X-Star [92] databases, is on photoionization and collision rate data. The transition probability material in these tables is mostly taken from other databases. The "Plasma-Gate" internet collection of atomic databases by Y. Ralchenko [151] provides a complete listing of all atomic databases.

Some active ongoing experimental and theoretical projects are:

(a) The FERRUM Project, which is an experimental effort to obtain highly precise f-values for Fe II. This has been recently reviewed in detail by S. Johansson [90].

(b) Emission (branching ratio) and lifetime measurements for rare-earth spectra, by J. Lawler et al. [61, 62, 63, 70, 104, 105, 106, 177], done with hollow cathodes and Penning discharges, and the laser-induced fluorescence method.

(c) Calculations and lifetime measurements of numerous rare-earth transitions, especially for singly- and doubly-charged ions, by Biemont, Garnir, Palmeri, Quinet, Svanberg, and co-workers [10, 11, 13, 14, 15, 18, 70, 111, 140, 141, 149, 187, 188, 189].

Also, the proceedings of the 7th International Colloquium on Atomic Spectra and Oscillator Strengths (ASOS 7) [87] contain several informative review articles on major recent work. We note that much of the ongoing activity has shifted to heavier elements, including the rare earths.

The remaining part 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. Table 1 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 immediately following this section. 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

RV — review articles

Table 1. Important Literature References

Ag I: 191	Ba I: 100, 101	Cl III: 78
Ag II: 26	Ba II: 100	Cl IV: 38
		Cl XII: 1
Al I: 175	Bi II: 139, 176	
Al II: 175	Bi III: 176	Co I: 134
Al VIII: 1		
Al XI: 168	C I: 5, 74, 107, 124, 190	Cu I: 191
	C II: 46, 127, 173, 190	Cu II: 20
Ar I: 150	C III: 127, 190	
Ar II: 72	C IV: 183, 190	Dy I: 177
Ar III: 64, 114		Dy II: 177
Ar IV: 64, 78	Ca I: 84, 115	
Ar V: 38	Ca IV: 165, 180	Er III: 10
Ar XIII: 1, 125		
	Cd III: 24	Eu I: 62
Au I: 191		Eu II: 62, 106, 193
Au II: 27, 155, 185	Ce I: 109	Eu III: 62, 117, 193
	Ce II: 109, 141, 188	
	Ce III: 109	F IV: 1

Table 1. Important Literature References (Continued)

Fe II: 69, 88, 93, 94, 107, 108, 132, 142, 156, 159, 164, 178
Fe III: 91
Fe V: 129, 130, 137
Fe VI: 43
Fe VIII: 9
Fe IX: 148
Fe X: 55, 56, 67, 121, 122, 148
Fe XI: 77, 148
Fe XII: 22, 148
Fe XIII: 126, 148
Fe XIV: 83, 121, 148
Fe XV: 2, 54
Fe XVI: 35
Fe XVIII: 184
Fe XX: 68
Fe XXI: 125
Fe XXIII: 42, 174
Fe XXV: 136

Gd II: 186
Gd III: 186

Ge I: 32, 110
Ge II: 32

He I: 118

Hg I: 146
Hg II: 31, 146, 157
Hg III: 146

Ho I: 63
Ho II: 63
Ho III: 18, 187

In II: 21

K III: 180

Kr II: 154
Kr IV: 33

La II: 104, 112, 194
La III: 15, 112

Lu I: 70
Lu II: 70, 149
Lu III: 15, 70

Mg V: 23

Mn II: 98, 99
Mn IX: 122

Mo II: 147, 163

N I: 124, 171, 192
N II: 103, 116, 169, 192
N III: 46, 173, 192
N IV: 192
N V: 192

Na III: 7, 120
Na VI: 1

Nd II: 144
Nd III: 28, 66, 189

Ne I: 58
Ne II: 59, 65
Ne III: 53

Ni II: 6, 71, 73, 76
Ni III: 128
Ni XVI: 8, 57, 83
Ni XVIII: 41

O I: 47, 124
O II: 60, 166, 167, 172
O III: 169
O IV: 46
O V: 96

P I: 78
P X: 1

Pb I: 3, 12, 52
Pb II: 3, 44
Pb III: 45

Pr II: 66, 89
Pr III: 13, 66, 140

Re II: 85

S I: 75, 181, 182
S II: 78
S IV: 80, 82, 86, 170
S V: 2, 81
S IX: 23, 25
S X: 95

Sc V: 180

Si II: 39, 119
Si III: 2
Si IV: 162
Si VI: 48
Si VII: 23
Si VIII: 95, 138
Si IX: 29, 169
Si X: 34
Si XI: 49
Si XII: 50
Si XIII: 50

Sm I: 153

Sn II: 4, 158

Sr II: 16

Ta II: 85, 135

Tb II: 61, 105
Tb III: 14

Th II: 133
Th III: 19

Ti II: 113, 143, 179
Ti XII: 37, 40

Tl II: 30

Tm II: 152
Tm III: 111

U II: 131

W II: 85, 97
W III: 160

Yb III: 11

Zr III: 36

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3. WORKING GROUP ON COLLISION PROCESSES
(GROUPE DE TRAVAIL POUR PROCESSUS DE COLLISIONS)

CHAIR: D.R. Schultz
CO-CHAIR: P.C. Stancil

Since the last working group report in 1999, very active research continues that spans the wide and deep 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 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 2002). 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 informantion. 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 using the following scheme: (1) electron impact of atoms and ions, (2) electron impact of molecules, (3) ion-atom and atom-atom collisions, (4) ion-molecule and atom-molecule collisions, and (5) reactive scattering and chemistry. Each of these sections contains a full range of reactions such as excitation, ionization, recombination, elastic scattering, *etc.*

3.1. Electron Impact of Atoms and Ions

Collisions of electrons with atoms and ions are the major excitation mechanism in astrophysical environments such as stellar atmospheres, planetary nebulae, and AGNs and, therefore, considerable effort continues to be devoted to such studies. These have included study of the following species: He (Beigman et al. 2000, Bray et al. 2000, Merabet et al. 2001), He^+ (Smith et al. 2001), Li (Schweinzer et al. 1999, Griffin et al. 2001), Li^+ (Brown, Scott, & Berrington 1999), C^{3+} (Greenwood et al. 1999, Janzen et al. 1999, Griffin, Badnell, & Pindzola 2000), O (Zatsarinny & Tayal 2001a, Kanik et al. 2001, Noren et al. 2001), O^+ (Tayal & Richardson 2000), O^{2+} (Niimura, Smith, & Chutjian 2002), O^{5+} (Griffin, Badnell, & Pindzola 2000, Lozano et al. 2001), O^{7+} (Berrington & Ballance 2002), N (Tayal & Beatty 1999), Ne^{2+} (McLaughlin & Bell 2000, McLaughlin, Daw, & Bell 2002), Al^{12+} (Aggarwal, Keenan, & Rose 2001), Si (Ganas 1999), Si^{2+} (Griffin et al. 1999a), S (Zatsarinny & Tayal 2001b), S^{2+} (Tayal & Gupta 1999, Smith et al. 2000), S^{3+} (Tayal 2000a), S^{14+} (Kimura et al. 1999), Ti^{22+} (Gupta, Deb, & Msezane 1999), Fe^+ (Burke et al. 2002), Fe^{2+} (McLaughlin et al. 2002), Fe^{5+} (Chen & Pradhan 1999a,b), Fe^{6+} (Berrington, Nakazaki, & Norrington 2000), Fe^{9+} (Tayal 2000b, Pelan & Berrington 2001), Fe^{10+} (Tayal 2000b), Fe^{12+} (Tayal 2000b), Fe^{13+} (Storey, Mason, & Young 2000), Fe^{14+} (Eissner et al. 1999a, Griffin et al. 1999a, Aggarwal et al. 1999), Fe^{15+} (Eissner et al. 1999, Bautista 2000), Fe^{16+} (Gupta, Deb, & Msezane 2000, Bhatia & Saba 2001, Beiersdorfer et al. 2001), Fe^{18+} (McLaughlin et al. 2001, Butler & Zeippen 2001a), Fe^{19+} (McLaughlin & Kirby 2001, Butler & Zeippen 2001b), Fe^{20+} (Aggarwal & Keenan 1999, Butler & Zeippen 2000, Badnell & Griffin 2001, Gu, M. et al. 2001), Fe^{21+} (Gu, M. et al. 2001, Badnell, Griffin, & Mitnik 2001), Fe^{22+} (Chidichimo et al. 1999, Chidichimo et al. 2000, Ballance, Badnell, & Berrington 2001, Gu, M. et al. 2001), Fe^{23+} (Gu, M. et al. 1999, Ballance, Badnell, & Berrington 2001, Gu, M. et al. 2001), Fe^{24+} (Fontes, Zhang, & Sampson 1999), Ni^{2+} (Bautista 2001), Ni^{4+} (Badnell & Griffin 1999, Burke et al. 2002), Ni^{11+} (Matthews et al. 1999), and Zn^+ (Zatsarinny & Bandurina 1999).

In addition, we note several studies involving series of ions, i.e. He-like ions (Whiteford et al. 2001, Li^+, C^{4+}, F^{7+}, Mg^{10+}, Griffin, Mitnik, & Pindzola 2001, and S^{14+}, Ca^{18+}, Fe^{24+}, Kimura et al. 2000); N-like ions (Zhang & Sampson 1999); and Mg-like ions (Si^{2+}, Ar^{6+}, Ti^{10+}, Fe^{14+}, Griffin et al. 1999b). Electron energy deposition in a gas of H, He, and H_2 has also been treated by Dalgarno, Yan, & Liu (1999).

Electron-impact ionization is important in determining the charge state balance of astrophysical plasmas or in determining energy loss of precipitating ions, for example. This highly studied area of atomic collision physics focuses most attention on energy and angle resolved probes of the underlying collision dynamics, but a number of works also continue to appear contributing needed data for under studied cases. For example, 1s ionization cross sections for H-, He-, Li-, and Be-like sequences have recently been computed (Fontes, Sampson, & Zhang 1999), scaling laws for ionization of hydrogenic ions have been considered (Stai, Fojon, & Rivarola 2000), and empirical formulas for ionization of ions (Bernshtam, Ralchenko, & Maron 2000) have been determined. In addition, new data for particular targets have appeared: He (Pindzola & Robicheaux 2000, Kim, Johnson, & Rudd 2000), Li (Schweinzer et al. 1999, Colgan et al. 2001), Li^+ (Brown, Scott, & Berrington 1999, Pindzola et al. 2000a), C (Pindzola et al. 2000b), C^{3+} (Mitnik et al. 1999, Scott, Teng, & Burke 2000, Teng et al. 2000, Badnell & Griffin 2000), Ne^{7+} (Riahi et al. 2001), as well as treatment of set of ions, e.g. single ionization of Fe^{4+}, Fe^{5+}, Fe^{6+}, Fe^{9+}, and Fe^{10+}, by Stenke et al. 1999a, and double ionization of Fe^+, Fe^{3+}, Fe^{4+}, Fe^{5+}, and Fe^{6+}, by Stenke et al. 1999b, and K-shell ionization of Cr, Ni, Cu, Sc, V by Gstir et al. 2001. A number of ionization cross sections for atoms and molecules can be found on-line at the National Institute of Standards and Technology (Kim et al. 2002).

New work considering radiative and dielectronic recombination have also appeared for the following species: Li^+ (Saghiri et al. 1999, Zhao & Shirai 2001a), C^{2+} (Davey, Storey, & Kisielius 2000), C^{3+} (Schippers et al. 2001), C^{4+} (Zhang, Nahar, & Pradhan 1999, Savin 1999, Zhao, Ichihara, & Shirai 2000, Xu et al. 2000, Zou et al. 2001), C^{5+} (Zhang, Nahar, & Pradhan 1999), O^{3+} (Kisielius & Storey 1999), O^{4+} (Moribayashi & Kato 1999), O^{6+} (Zhao & Shirai 2001b), O^{7+} (Zhang, Nahar, & Pradhan 1999, Savin 1999), N^+ (Kisielius & Storey 2002), N^{4+} (Glans et al. 2001), Fe^{16+} (Donnelly et al. 1999, Zhang, Nahar, & Pradhan 2001), Fe^{22+} (Moribayashi & Kato 1999), Fe^{24+} (Zhang, Nahar, & Pradhan 1999, Watanabe, H. et al. 2001), and Ni^{25+} (Schippers et al. 2000).

Elastic scattering of electrons from ions and atoms can be important in determining transport properties of plasmas/gases and we note new work for He and other noble gases by Zubek et al. (1999) and for O by Zatsarinny & Tayal (2001a).

3.2. Electron Impact of Molecules

Electron impact of molecules is an important process in many relatively dense environments such as planetary atmospheres and nebulae. These processes can be important through line excitation and cooling. Recent studies of excitation of molecules include H_2O (Moreira, Thompson, & McLaughlin 2001), CO (Beegle et al. 1999), CO_2 (Eustatiu et al. 2000), O_2^+ and TiO^+ (Ballance, Berrington, & McLaughlin 1999), N_2 (Campbell et al. 2001, Odagiri et al. 2001), N_2^+ (Nagy et al. 1999), and NO^+ (Rabadan & Tennyson 1999).

New data for ionization can be found for H_2 (Kim & Rudd 1999, Celiberto et al. 1999, Hanel et al. 2002), H_2O (Kim & Rudd 1999, Hanel et al. 2002, Champion, Hanssen, & Hervieux 2002), CO (Tian & Vidal 1999, Almeida et al. 1999, Mangan, Lindsay, & Stebbings 2000), CO_2^+ (Deutsch et al. 2002), CH_4 (Khare, Sharma, & Tomar 1999), C_2H_2 (Furuya et al. 2000), N_2^+ (Deutsch et al. 2002), NO (Lindsay et al. 2000), NO_2 (Lindsay et al. 2000, Jiao et al. 2002), and for dissociative ionization of O_2^+ and N_2^+ (Siari et al. 1999), NH_2^+, NH_3^+, NH_4^+, OH_2^+, and OH_3^+ (Djuric et al. 2000), CO_2^+ (Bahati et al. 2001a), and N_2^+ (Bahati et al. 2001b). We note that dissociative excitation has been considered for H_2 (Celiberto et al. 1999).

The process of dissociative recombination is an important process in which the electron is captured by a molecular ion resulting in a number of neutral products. It is an efficient process producing complex neutral molecules: H_2^+ (Larson et al. 2000, Serov et al. 2001, Pichl, Nakamura, & Horáĉek 2001), HD^+ (Amitay et al. 1999, Larson et al. 2000, Orel 2000, Larson & Orel 2001), H_3^+ (Jensen et al. 2001, Glosík et al. 2001, Strasser et al. 2001a,b), H_2O^+ (Jensen et al. 1999), H_3O^+ (Neau et al. 2000, Bahati et al. 2001c), HCN^+ (Sheehan et al. 1999, Talbi, LePadellec, & Mitchell 2000), He_2^+ (Carata, Orel, & Suzor-Weiner 1999), HeH^+ (Larson & Orel 1999), LiH^+ (Krohn et al. 2001), CH^+ (Carata et al. 2000), $C2H_2^+$ (Derkatch et al. 1999), OH^+ (Larson et al. 2000), O_2^+ (Peverall et al. 2001), and NO^+ (Mostefaoui et al. 1999, Schneider et al. 2000, LePadellec et al. 2001).

We also note new data for dissociative attachment of H_2 and it isotopes (Orient & Chutjian 1999, Xu, Gallup, & Fabrikant 2000, Xu, Kazansky, & Fabrikant 2001, Xu & Fabrikant 2001), Li_2 (Pozdeev 1999), O_3 (Rangwala et al. 1999), and for elastic scattering from N_2 (Lee & Iga 1999, Garcia & Blanco 2001), CO (Garcia & Blanco 2001), CO_2 (Gianturco & Stoecklin 2001), O_2 (Machado et al. 1999, Raj & Kumar 2001), CO_2 (Rescigno et al. 1999), NO (Fujimoto & Lee 2000), NO_2 (Curik et al. 2001), and H_2O (Ingr et al. 2000).

3.3. 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 D^+ (Esry et al. 2000, Savin 2002), C^{2+} (Errea et al. 2000c), C^4+ (Belyaev et al. 2002), S^{4+} (Stancil et al. 2001), and Cl^{7+} (Thompson et al. 2001), and on H^+ include Li (Salas 2000), O (Stancil et al. 1999), Na (Dutta et al. 2001), and Mg (Amaya-Tapia, Hernández-Lamoneda, & Martínez 2001). He is also an important target where studies have considered the incident ions He^{2+} (Rabli, Gargaud, & McCarroll 2001), $Be^{(1-4)+}$ (Suzuki et al. 2000), O^{2+} (Itoh 2002), F^{2+} (Gu, J.-P. et al. 2000), Al^{2+} (Watanabe, A. et al. 2001), and Si^{4+} (Vacek et al. 2001). On-line databases include the National Institute for Fusion Science (NIFS) Charge Transfer Database Chart (2002) and the ORNL/UGA Charge Transfer Database for Astrophysics (2002) sites.

Molecules can be formed by collisions of atoms and ions through radiative association. Dickinson and Gadéa (2000) considered formation of LiH by collisions of Li^+ with H^-. Other recent results include radiative association formation of SiH^+, PH^+, and SH^+ (Stancil et al. 2000) and CH_5^+ (Bacchus-Montabonel, Talbi, & Persico 2000).

3.4. Ion-Molecule and Atom-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 $H^+ + H_2$ (Kusakabe et al. 2000), C^{4+} (Errea et al. 2002a), C^{4+}, N^{5+}, O^{6+} (Lubinski et al. 2000), and $O^{(5-8)+}$ (Liu & Schultz 1999) with H_2; H^+ (Kimura et al. 2000; Ĉadeẑ et al. 2002), He^+ (Ĉadeẑ et al. 2002; Kwong, Chen, & Fang 2000), He^{2+} (Kearns et al. 2001), C^+ (Lu et al. 2000), $O^{(2-5)+}$ (Gao, Fang, & Kwong 2001; Gao & Kwong 2002) with CO; He^+ with N_2 and CH_4 (Fang, Chen, & Kwong 2000); $Ne^{(3,4)+}$ with N_2 and O_2 (Kamber & Ferguson); Co^{3+} with N_2 (Gao et al. 2002); O^+ with NO (Levandier, Chiu, & Dressler 2000); and H^+ and $He^{(1,2)+}$ with H_2O and CO_2 (Greenwood et al. 2000a). In addition for applications to x-ray emission from comets a number of investigations have considered a range of highly charged ions on various molecular targets: C, N, O, and Ne from 3+ to 10+ on H_2O, CO_2, H_2 and He (Greenwood et al. 2000b; 2001); N^{7+} and O^{7+} on H_2O, CO, CO_2, and He (Hasan et al. 2001); and Si^{13+}, S^{15+}, and Ar^{17+} on H_2, CO, CO_2, CH_4, and O_2 (Tawara et al. 2001).

In some environments, advances in modeling require vibrationally-resolved charge transfer data. Such data are generally not available, but some studies have recently been performed for $H^+ + H_2$ (Ichihara, Iwamoto, & Janev 2000; Ichihara, Iwamoto, & Yokoyama 2001; Krstić, Schultz, & Janev 2002) and $C^{2+} + H_2$ (Errea et al. 2000b).

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_2 (Flower 2000); CO by H (Balakrishnan, Yan, & Dalgarno 2002), He (Zhu, Balakrishnan, & Dalgarno 2001; Cecchi-Pestellini et al. 2002), and H_2 (Flower 2001); and CH_3OH by He (Pottage, Flower, & Davis 2002).

Tabata & Shirai (2000) present a compilation of analytical fits for a variety of processes for collisions of H^+, H_2^+, H_3^+, H, H_2, and H^- with H_2 while Wang & Stancil (2002) have compiled the available $H^+ + H_2$ isotopomer collision data.

3.5. Reactive Scattering and Chemistry

Due to space limitations, we cannot review the many and exciting advances in chemical processes and reactive scattering relevant to astrophysics. However, we refer the reader to a number of compilations and review articles. The UMIST astrochemistry database was updated to include 4113 gas-phase reactions important for interstellar and circumstellar chemistry (Le Teuff, Millar, & Markwick 2000). Lepp, Stancil, & Dalgarno (2002) have reviewed chemistry in the early Universe and primordial clouds and provide some updated reaction rate coefficients. Of interest to Li chemistry are reactive scattering studies in the LiH_2 (Dunne et al. 2001; Bodo et al. 2001a) and LiH_2^+ (Bodo et al. 2001b) systems. Talbi & Herbst (2002) have investigated destruction reactions of CO_2 by H and H_2. Other reactions of interest include $Cl + H_2$ (Manthe, Bian, & Werner 1999) and $OH + H_2$ (Troya et al. 2001; Rodríguez et al. 2001).

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4. WORKING GROUP ON LINE BROADENING
(GROUPE DE TRAVAIL POUR LES PROFILS DE RAIES)

CHAIR: C. STEHLE
CO-CHAIR: G. PEACH

The period from 1999 to 2002 has been marked by two International Conferences on Spectral Line Shapes in Berlin (2000) and in Stanford (2002), and the publication of the bibliography on Atomic Line Shapes and Shifts for the period from 1989 to 1999 (Konjević et al. 2001). The report will be divided into two parts, Stark and neutral broadening respectively, and we shall focus our attention on results which are the most relevant to astrophysics.

4.1. Stark Broadening

In this field, we note the recent review of Konjević (1999) on the plasma broadening and shift of non-hydrogenic lines. Helpful formulas are given that can be used for astrophysical applications, and are particularly useful when data for electron-impact widths and shifts do not exist.

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 plasma electrons. In this field, semi-classical or semi-empirical theories are the most popular, because of their simplicity and accuracy, of about 20 % on average. In addition to recent numerical developments (Rivière 2002), the new feature is the increasing number of predicted and measured line widths. Experiments are mostly performed in Spain, Serbia and Poland in which the electronic density is around 10^{17} cm^{-3} and temperatures are between 10,000 K and 20,000 K.

These experiments have produced data on the widths (and shifts) of lines in Kr II, Kr III (de Castro et al 2001, Milosavljević et al. 2000), C II, C III and C IV (Srećković et al. 2000), N II (Mar et al. 2000), Ar I (Aparicio et al. 1998), Ar IV (Djenize et al. 2001), Ne

II (Djenize et al. 2002), Ne II, Ne III and Ne IV (Milosavljević et al. 2001), Br I (Bacławski et al. 2002), C III, N III, O III, F III, Ne III (Blagojević et al. 2000), O III (Srecković et al. 2001), Si III (Gonzalez, et al. 2000), Sn I and Sn II (Martínez and Blanco 1999), Xe III (Seidel et al. 2001), Zr II, Zr III (Dimitrijević et al. 2001). Regularities in the widths of neutral *ns*-*np* and *np*-*ns* lines have been investigated by Sarandaev et al. (2000), and an interesting study of the line of N I at 791.5 nm has been carried out in order to obtain very accurate results for use in future measurements of electron densities (Wujec et al. 2002).

This renewal of experimental studies is matched by theoretical calculations, as for example for Pb II (Colon et al. 2002) , Nd II (Popović et al. 2001), Cu I (Il'in et al.), Ag II (Tankosić et al. 2001) and also by detailed analyses of lines of N I, O I, N II and O II (Rivière 2002).

Hydrogen lines

The new developments are also mostly experimental with several studies of hydrogen lines at high densities (i.e., between 10^{17} cm^{-3} and 10^{19} cm^{-3}) performed either in high pressure H_2 cells subjected to CO_2 laser light (Bock et al. 2001), or in a linear flash tube at high pressure (Flih and Vitel 2001), in underwater laser plasmas (Escarguel et al. 2000 a, b), and in a gas liner pinch (Buscher et al. 2002). These studies are necessary to improve the knowledge of hydrogen line broadening at high densities where short-range interactions modify the line shape and produce an asymmetry and a noticeable shift.

In addition, theoretical work on this difficult topic has been carried out using either computer simulations (Olchawa 2002), or the Model Microfield Method (MMM) (Stehlé et al. 2000 a, Sorge and Gunter, 2000). All these developments are exploratory. In this density regime, the study by computer simulation of Ly_α,Ly_β, H_α, H_β, in the dipole approximation (Halenka et al. 2002), indicates a very small effect of the perturber charges for a given electronic density. But at high density (N_e about 10^{19} cm^{-3}) a delicate experiment in the red line wing of H_α indicates the presence of a molecular H^+ - H satellite that is predicted by the theory (Kielkopf et al. 2002). New theoretical developments have been incorporated in a recent study of the line wings of Ly_β (Allard et al. 2000).

At low electron densities, the tabulations of the line shape of Ly_α for one and two photons using computer simulation (Gonzalez and Gigosos 2000) illustrate the effects of fine structure and ion dynamics, both calculated in the line centre to a very high accuracy.

An emerging topic is the study of hydrogen lines in magnetized plasmas which is important for the analysis of both stellar atmospheres and tokamak plasmas (Stehlé et al. 2000 a, Godbert-Mouret et al. 2001). Also the first calculation of polarized line shapes (Stehlé et al. 2000 b) is relevant to the determination of the magnetic field in stellar atmospheres.

Lines of one-electron ions

For the Lyman series of He II, we report a gas liner experiment at 10^{18} cm^{-3} (Wrubel et al. 2001). The study of these lines, especially in the high density regime, still represents a considerable theoretical challenge. A theoretical study of line asymmetry and shift using MMM theory and the computation of dipole profiles of Lyman and Balmer lines using computer simulations have been carried out (Halenka et al. 2002).

Neutral Helium lines

We note two experimental studies, one at 10^{18} cm^{-3} for the line at 587 nm and another at lower density (4×10^{16} cm^{-3}) for the transition at 447.1 nm at temperatures of the order of 20,000 K (Milosavljević and Djenize 2001, Bardet et al. 2002).

4.2. Broadening by neutral atoms and molecules

Developments in lineshape theory

There has been an increasing realisation that in the analysis of spectral lineshapes it is often important to allow for departures from the usual Voigt profile. An algorithm

for calculating a speed-dependent Lorentzian profile which is computationally efficient has been developed by Berman et al. (1999), and Robert et al. (2000) have produced a velocity-memory model for the spectral lineshape from the Doppler to the collision regime. Ciuryło and Pine (2000) have developed spectral profiles of overlapping lines for speed-dependent broadenings, shifts and couplings. Doppler broadening and Dicke narrowing are incorporated in the analysis of atmospheric spectra, and Pine and Ciuryło (2001) have tested their generalised theory by applying it to multispectrum fits for HF broadened by Ar. Parker (2001) has studied line mixing effects in CO_2 broadened by air, and D'Eu et al. (2002) have used infrared HCN lineshapes as a test of Galatry and speed-dependent Voigt profiles for broadening by the rare gases, N_2, HCN and CH_3Br.

Broadening of atomic lines

Barklem et al. (2000a) and Barklem et al. (2000b) have studied the self-broadening of hydrogen lines, and an analysis of Balmer wing formation in the solar spectrum improves agreement with observation but still leaves discrepancies. Theoretical studies of the broadening of Na lines by H and He have been made by Barklem and O'Mara (2001), Leininger et al. (2000), Stoker et al. (2002) and Leo et al. (2000). Barklem and O'Mara (2000) and Barklem et al. (2000c) have produced data for the broadening by hydrogen of many lines of the elements Li–Ni that are of astrophysical importance. The data are listed in the Strasbourg and Vienna databases (see below).

Broadening of molecular lines

Much experimental data has been published in the period 1999-2002. The molecules are listed below with their perturbing atomic or molecular species.

CO broadened by He, H_2, CO, CO_2, N_2, O_2 and H_2O. Henningsen et al. (1999), Predoi-Cross et al. (1999), Priem et al. (2000b), Mantz et al. (2001), Di Rosa and Farrow (2001) and Devi et al. (2002d).

CO_2 broadened by CO_2, N_2 and air. Henningsen and Simonsen (2000), Parker (2001), Devi et al. (2002e,f).

O_2 broadened by CO, CO_2, N_2, O_2, and SF_6. Amano et al. (1999), Pope et al. (2000) and Cheah et al. (2000).

O_3 broadened by N_2, O_2, O_3, and air. Priem et al. (2000a) and Larsen et al. (2001).

OH and NO broadened by He. Hübers et al.(1999).

NO broadened by the rare gases, N_2 and O_2. Pope and Wolf (2001) and Colmont et al. (2001).

NO_2 broadened by N_2 and air. Voigt et al. (2002) and Vandaele et al. (2002).

H_2O broadened by the rare gases, N_2, O_2, H_2O, and air. Moretti et al. (2001), Claveau et al. (2001) and Steyert et al. (2002).

NH_3 broadened by He, Ar, H_2 and NH_3. Hadded et al. (2001), Bouanich et al. (2001) and Baldacchini et al. (2000).

HNO_3 broadened by N_2, O_2, and HNO_3. Zu et al. (2002).

CH_4 broadened by H_2. Hartmann et al. (2002).

CS_2 broadened by O_2, N_2, and air. Lengelé et al. (2002).

C_2H_2 broadened by He and N_2. Blanquet et al. (2001).

SO_2 broadened by SO_2. Sumpf (2001).

CH_3D broadened by CH_3D, N_2 and air. Devi et al. (2002a,b,c), Devi et al. (2000) and Devi et al. (2001a,b).

Collision-induced spectra

Theoretical studies of collision-induced spectra for H_2-H_2 pairs have been carried out by Brodbeck et al. (1999), Fu et al. (2000), Borysow et al. (2000) and Borysow et al. (2001). These spectra are important for the modelling of the atmospheres of planets and cool stars.

Transitions in CO_2 produced by H_2, N_2 and O_2 have also been studied theoretically by Brown et al. (2000) and Brown and Tipping (2001).

Databases

A 'virtual observatory' is being 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 a new version of the database High resolution Transmission, HITRAN2000, can be found at:

http://www.hitran.com.

The current version of the database Gestion et Etude des Informations Spectroscopiques Atmosphériques (GEISA-97) 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,

and the Vienna Atomic Line Database (VALD) can be found at:

http://www.astro.univie.ac.at/~ vald.

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5. WORKING GROUP ON MOLECULAR STRUCTURE
(GROUPE DE TRAVAIL POUR LA STRUCTURE MOLECULAIRE)

CHAIR: E.F. VAN DISHOECK
CO-CHAIR: J.H. BLACK

The literature on molecular structure, spectra, and transition data is vast. Only some of the published work is potentially relevant to astrophysics. Even so, this brief review can cover only a fraction of the relevant work. It is notable that the Astrophysical Data System (ADS) Abstract Service has recently been expanded to include a larger sample of journals in physics and chemical physics that publish articles on molecular structure and spectra. Interested readers are encouraged to use this valuable resource at

`http://adsabs.harvard.edu/abstract_service.html`

or one of its mirror servers.

During the reporting period, international meetings have been devoted to astrophysically interesting molecules H_2 (Combes & Pineau des Forêts 2000) and H_3^+ (Herbst et al. 2000).

5.1. Fundamental Data and Databases

In addition to the well known JPL (`http://spec.jpl.nasa.gov`) and Lovas (`http://physics.nist.gov/PhysRefData/ micro/html/contents.html`) databases on molecular spectroscopy, the microwave spectroscopy group in Cologne has published an extensive and growing database (`http://www.ph1.uni-koeln.de/ vorhersagen/index.html`; see Müller et al. 2001). A database relating to high-resolution molecular spectroscopy is maintained by E. Hirota (`http://aci.soken.ac.jp/database/molecular/top.html`). Bernath & McLeod (2001) have brought the bibliographical catalogue of diatomic molecular spectra of Huber & Herzberg into the 21st century through a database at

`http://diref.uwaterloo.ca/`.

5.2. Electronic Spectra

The discovery of a forbidden electronic transition $a^1\Delta - X^3\Sigma^-$ of SO in the infrared spectrum of Io has been reported (de Pater et al. 2002), based upon recent laboratory spectroscopy (Setzer, Fink & Ramsay 1999). Isotope abundances of Mg in sunspots have been measured through use of several bands of the MgH $B'\ ^2\Sigma^+ - X^2\Sigma^+$ system (Wallace et al. 1999). Watson (2001) has re-examined old laboratory spectra of CH to identify three interstellar absorption lines near 136.9 nm with the $3d - X^2\Pi$ transition of that radical.

Quantitative spectroscopy of carbon monoxide and its isomers continues to advance. Lifetimes as long as 0.1 s have been measured for individual levels of the metastable $a^3\Pi$ state (Sykora & Vidal 2000). Triplet Rydberg states of CO have been investigated with a far-UV laser light source (Mellinger, Rohwer & Vidal 2001) and forbidden triplet-singlet transitions have been studied by conventional absorption spectroscopy (Baker et al. 2000; Rostas et al. 2000; Stark et al. 2002; Eidelsberg & Rostas 2002). New oscillator strengths have been reported for the B–X, C–X, and E–X transitions of CO (Federman et al. 2001). Predissociations in the $E^1\Pi$ (Ubachs & Velchev 2000) and $C^1\Sigma^+$ (Cacciani et al. 2001) states of CO have been investigated.

The hydrogen molecule continues to attract spectroscopic attention. High-resolution electron-impact emission spectroscopy has been reported (Jonin et al. 2000; Liu et al. 2000; Liu et al. 2002). New data on the total transition probabilities and spontaneous radiative dissociation of H_2 in its B, C, B′, and D states have been published (Abgrall, Roueff & Drira 2000). *Ab initio* calculations of electronic transition moments for a number of singlet and triplet transitions in H_2 have been presented (Drira 1999).

Photodissociation of HCN and DCN by H I Lα radiation has been investigated through use of the technique of Rydberg atom time-of-flight spectroscopy (Cook et al. 2000). A new study of photodissociation of H_2O below 132 nm has been carried out (Zanganeh et al. 2000) in which the vibrational and rotational distributions of product OH have been determined, and the experimental results have been compared with new three-dimensional quantum mechanical calculations (van Harrevelt et al. 2001; Fillion et al. 2001).

Work on the electronic spectra of carbon-chain molecules, which was partly stimulated by interest in identifying the diffuse interstellar bands, has received new impetus from the identification of C_3 in the interstellar medium (Maier et al. 2001). Searches for larger carbon molecules like C_4 and C_5 (Maier, Walker & Bohlender 2002) have been made possible by laboratory investigations of the gas-phase electronic spectra of these (Linnartz et al. 2000; Motylewski et al. 1999) and related (C_3H: Ding et al. 2001; $C_3H_2^-$: Güthe et al. 2001; HC_6N: Vaizert et al. 2001; C_7^-: Lakin et al. 2000) species.

Far-ultraviolet spectroscopic data on N_2 are of interest for studies of occultations of planetary atmospheres: new results have been published by Stark et al. (2000) and added to an associated data archive (`http://cfa-www.harvard.edu/amdata/ampdata/N2ARCHIVE/n2home.html`). Radiative lifetimes of Rydberg states of N_2 have been determined through use of a picosecond XUV laser (Ubachs et al. 2001).

Doppler-limited spectroscopy has been carried out on O_2 and NO through use of a vacuum-ultraviolet Fourier transform spectrometer (Yoshino et al. 2000a,b; Imajo et al. 2000; Rufus et al. 2001; Cheung et al. 2002).

5.3. Vibrational Spectra

Much effort has gone into refining the vibrational energy level structure of the water molecule H_2O: see Bernath (2002) for a review and Tennyson et al. (2001) for a tabulation of experimental energy levels. This work has led, for example, to the identification of hot water in sunspot spectra (Zobov et al. 2000). A sensitive, high-resolution infrared spectrograph developed for astronomical observations has also applied to laboratory spectroscopy of NH and improved, extended molecular constants have resulted (Ram, Bernath & Hinkle 1999).

5.4. Rotational Spectra

In the last 3 years, a wealth of new spectroscopic data on microwave transitions of carbon-chain molecules and exotic rings has been obtained, primarily in the CfA laboratory led by P. Thaddeus and M. McCarthy. New spectra include those of polyyne chains (McCarthy et al. 2000b, Gordon et al. 2000, Tang et al. 2001), cumulene carbenes (Apponi et al. 2000a, McCarthy & Thaddeus 2002), Si-containing chains (Apponi et al. 2000b, McCarthy et al. 2000a), S-containing chains (Gordon et al. 2001, 2002), and cyclic species (Apponi et al. 2001). Laboratory spectroscopy is now well ahead of radio astronomy in the detection of new species.

Rotational spectra of many metal-containing molecules that may exist in the envelopes around late-type stars and possibly in interstellar clouds have been measured primarily by L. Ziurys' group. Recent results include the spectra of KH (Brewster & Ziurys 2001a), $MgNH_2$ (Sheridan & Ziurys 2000), NiC and CoC (Brewster & Ziurys 2001b), NiCl (Yamazaki et al. 2001), CuS and MnS (Thompsen & Ziurys 2001; Thompsen et al. 2002), and NaC (Sheridan et al. 2002). Astronomical searches for these species are pursued and the detection of AlNC has recently been reported (Ziurys et al. 2002).

With the increased interest in searches for pre-biotic molecules, additional molecular data on the spectra of complex organic molecules are needed. De Lucia, Herbst and co-workers have provided new data on glycolaldehyde CH_2OHCHO (Butler et al. 2001), acetone CH_3COCH_3, methyl-ethyl ether $CH_3OC_2H_5$, and methyl carbamate $H_2NCOOCH_3$ (Herbst et al. 2002), whereas Habara & Yamamoto (2001) have measured CH_3CCS. Rotational

spectra of HC_3N in the ground and vibrationally excited states have been obtained by Thorwirth et al. (2000b).

With new far-infrared missions such as SOFIA and Herschel on the horizon, terahertz spectroscopy of astrophysically relevant species is gaining in importance. The laboratory focus is on small species such as H_2O (Chen et al. 2000), CH (Davidson et al. 2001), CF (Morino et al. 2000), C_2H (Müller et al. 2000a), HNC (Thorwith et al. 2000c), HCN (Maiwald et al. 2000), C_3 (Giesen et al. 2001), NH_2 (Gendriesch et al. 2001) and PH_2 (Margules et al. 2002), but terahertz data on more complex molecules like CH_3C_2H (Müller et al. 2000b) and ethylenimine c-C_2H_4NH (Thorwirth et al. 2000a) are appearing as well.

An improved model for the millimeter and submillimeter atmospheric transmission which includes the latest spectroscopic data has been published by Pardo et al. (2001) and tested against observational data.

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6. WORKING GROUP ON MOLECULAR REACTIONS ON SOLID SURFACES

(GROUPE DE TRAVAIL POUR REACTIONS MOLECULAIRES SUR LES SURFACES SOLIDES)

CHAIR: W.A. SCHUTTE
CO-CHAIR: L.B. D'HENDECOURT

6.1. Introduction

The study of the role of dust in interstellar chemistry has progressed in a number of ways over the last 3 years. Experimental studies have further clarified the role that dust may play in the formation of the simple saturated molecules that are observed in the ISM, by simulating the catalytic chemical processes on the surface. In addition, the application of chemical analysis techniques such as gas chromatography/mass spectroscopy and time-of-flight mass spectroscopy opened a new window on the chemistry ot the processing of ices by UV and particles by the identification of a suite compounds, some of which could be of astrobiological relevance. Important progress was also made in the characterization of the ices on the bodies in the outer solar system. Detailed matches of the NIR absorption bands in the spectrum of Triton could be achieved by a combination of experimental production of ice analogs and modelling of the influence of the surface texture. A very promising development is the identification and direct study of interstellar grains in interplanetary dust particles and primitive meteorites. The study of the isotopic composition of such grains can be used to trace their origin in stars or in the ISM. A new approach arose in the efforts of modelling phenomena caused by interstellar dust (e.g., extinction, emission, absorption bands). This generally involves limiting as much as possible any a priori constraints on the dust properties, and modelling the observations in the most general way possible, to get an unbiased picture of the constraints set by the observations. Another "first" is the use of quantum mechanical calculations to predict reactions that may occur in interstellar or

solar system ices. This tool, in combination with the results from laboratory experiments, could lead to a better understanding of interstellar solid state chemistry.

6.2. Reviews and Meetings

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Solid Interstellar Matter: The ISO Revolution, Les Houches Workshop, February 2-6, 1998. Edited by L. d'Hendecourt, C. Joblin, and A. Jones. EDP Sciences and Springer-Verlag (1999).

6.3. Properties of Interstellar Dust Grains

The Ortho/Para Ratio of H_2 Newly Formed on Dust Grains (Takahashi 2001); Processing of silicate dust grains in Herbig Ae/Be systems (Bouwman et al. 2001); Photoelectric effect on dust grains across the L1721 cloud in the rho Ophiuchi molecular complex (Habart et

al. 2001); Evidence for Dust Grain Growth in Young Circumstellar Disks; implications for the formation rate of planetary systems (Throop et al. 2001); Photoelectric Emission from Interstellar Dust: Grain Charging and Gas Heating (Weingartner & Draine 2001); Infrared Emission from Interstellar Dust. I. Stochastic Heating of Small Grains (Draine & Li 2001); Infrared Emission from Interstellar Dust. II. The Diffuse Interstellar Medium (Li & Draine 2001); Interstellar extinction by composite grains (Vaidya et al. 2001); Modified rate equations revisited. A corrected treatment for diffusive reactions on grain surfaces (Stantcheva et al. 2001); New models of interstellar gas-grain chemistry - II. Surface photochemistry in quiescent cores (Ruffle & Herbst 2001); New models of interstellar gas-grain chemistry - I. Surface diffusion rates (Ruffle & Herbst 2000) New models of interstellar gas-grain chemistry - III. Solid CO_2 (Ruffle & Herbst 2001); Study of the Reactions of H and D Atoms with Solid C_2H_2, C_2H_4, and C_2H_6 at Cryogenic Temperatures (Hiraoka et al. 2000); The Composition and Distribution of Dust Along the Line of Sight Towards the Galactic Center (Chiar et al. 2000); Reaction of H Atoms with Solid C_2H_4 and C_2H_6 at 13 K (Hiraoka et al. 1999); Extended D2CO emission: The smoking gun of grain surface-chemistry (Ceccarelli et al. 2001); Master Equation for Hydrogen Recombination on Grain Surfaces (Biham et al. 2001); The effect of the initial elemental abundance on gas-grain chemical models (Shalabiea 2001); Accretion Disks around Young Objects. III. Grain Growth (D'alessio et al. 2001); X-Ray Halos and Large Grains in the Diffuse Interstellar Medium (Witt et al. 2001); On Ultrasmall Silicate Grains in the Diffuse Interstellar Medium (Li & Draine 2001); Low-temperature crystallization of silicate dust in circumstellar disks (Molster et al. 1999); The chemical composition of the silicate dust around RAFGL7009S and IRAS 19110+1045 (Demyk et al. 1999); On the Model of Dust in the Small Magellanic Cloud (Zubko 1999); The formation mechanism of molecular hydrogen on icy mantles of interstellar dust (Takahashi et al. 1999); Grain Surface Recombination of HCO+ (Aikawa et al. 1999); Calculating Cross Sections of Composite Interstellar Grains (Voshchinnikov & Mathis 1999); The temperature of non-spherical interstellar grains (Voshchinnikov et al. 1999); Dust Grain-Size Distributions and Extinction in the Milky Way, Large Magellanic Cloud, and Small Magellanic Cloud (Weingartner et al. 2001); Circular polarization by scattering from spheroidal dust grains (Gledhill & McCall 2000); Aspects of the mass distribution of interstellar dust grains in the solar system from in situ measurements (Landgraf 2000); Dust around Herbig Ae/Be Stars: Porous, Cometary-Like Grains? (Krivova and Il'in 2000); Dust Coagulation in Infalling Protostellar Envelopes. I. Compact Grains (Suttner et al. 1999), Molecular Hydrogen Formation on Astrophysically Relevant Surfaces (Katz et al. 1999).

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Optical properties of the carbon dust grains in the envelopes around asymptotic giant branch stars (Suh 2000); Modeling of C stars with core/mantle grains: Amorphous carbon + SiC (Lorenz-Martins et al. 2001); Activation of the 3.4 Micron Band in Carbon Grains by Exposure to Atomic Hydrogen (Mennella et al. 1999); UV photodestruction of CH bonds and the evolution of the 3.4 mu m feature carrier. II. The case of hydrogenated carbon grains (Mennella et al. 2001); Infrared Spectroscopy of Nano-sized Carbon Grains Produced by Laser Pyrolysis of Acetylene: Analog Materials for Interstellar Grains (Schnaiter et al. 1999); Measurements of molecular hydrogen formation on carbonaceous grains (Pirronello et al. 1999); The use of kerogen data in understanding the properties and evolution of interstellar carbonaceous dust (Papoular 2001); Evolution of Carbon Dust in Aromatic Infrared Emission Sources: Formation of Nanodiamonds (Duley & Grishko 2001); Circumstellar Carbonaceous Material Associated with Late-Type Dusty WC Wolf-Rayet Stars (Chiar & Tielens 2001); Dust formation in carbon-rich Wolf-Rayet stars. I. Chemistry of small carbon clusters and silicon species (Cherchneff et al. 2000); ISO observations of the reflection nebula Ced 201: evolution of carbonaceous dust (Cesarsky et al. 2000); Carbonaceous onion-like particles as a component of interstellar dust (Wada et al. 1999); The Structure of Carbonaceous Dust Grains and the 2175 Angstroms Feature (Will & Aanestad 1999);.

6.5. Astrophysical Ices

Solid Carbon Dioxide in Regions of Low-Mass Star Formation (Nummelin et al. 2001); Searching for Ammonia in Grain Mantles toward Massive Young Stellar Objects (Gibb et al. 2001); Oservational Constraints on the Abundance and Evolution of "XCN" in Interstellar Grain Mantles (Whittet et al. 2001); Further evidence for the assignment of the XCN band in astrophysical ice analogs to OCN^-. Spectroscopy and deuterium shift (Novozamsky et al. 2001); Carbon Suboxide in Astrophysical Ice Analogs (Gerakines & Moore 2000); Production of Hexamethylenetetramine in Photolyzed and Irradiated Interstellar Cometary Ice Analogs (Cottin et al. 2001); Thermal desorption of water ice in the interstellar medium (Fraser et al. 2001); Ice absorption features in the 5-8 μm region toward embedded protostars (Keane et al. 2001); The Photostability of Amino Acids in Space (Ehrenfreund et al. 2001); Bands of solid CO_2 in the 2-3 mu m spectrum of S 140:IRS1 (Keane et al. 2001); Cold H_2O and CO Ice and Gas toward the Galactic Center (Moneti et al. 2001); The Formation of Cyanate Ion (OCN-) in Interstellar Ice Analogs (Hudson et al. 2001); Formation of Carbon Dioxide by Surface Reactions on Ices in the Interstellar Medium (Roser et al. 2001); The Abundances of Solid N_2 and Gaseous CO_2 in Interstellar Dense Molecular Clouds (Sandford et al. 2001); Laboratory Measurements of Molecular Hydrogen Formation on Amorphous Water Ice (Manic et al. 2001); Search for NH3 ice in cold dust envelopes around YSOs (Dartois & d'Hendecourt 2001); The obscured mid-infrared continuum of NGC 4418: A dust- and ice-enshrouded AGN (Spoon et al. 2001); Ab Initio Quantum Chemical Studies of Reactions in Astrophysical Ices. 2. Reactions in H2CO/HCN/HNC/H2O Ices (Woon 2001); Measurements of D2 Yields from Amorphous D2O Ice by Ultraviolet Irradiation at 12 K (Watanabe et al. 2000); H, C, N, and O Isotopic Substitution Studies of the 2165 Wavenumber (4.62 Micron) "XCN" Feature Produced by Ultraviolet Photolysis of Mixed Molecular Ices (Bernstein et al. 2000); Infrared spectra of CO_2 in H_2O:CH_3OH:CO_2 icy mixtures (Palumbo & Baratta 2000); Infrared observations of hot gas and cold ice toward the low mass protostar Elias 29 (Boogert et al. 2000); Deuterium Enrichment of Polycyclic Aromatic Hydrocarbons by Photochemically Induced Exchange with Deuterium-rich Cosmic Ices (Sandford et al. 2000); An Inventory of Interstellar Ices toward the Embedded Protostar W33A (Gibb et al. 2000); 1-4 Micron Spectrophotometry of Dust in the Taurus Dark Cloud: Water Ice Distribution in Heiles Cloud 2 (Murakawa et al. 2000); New experiments and interpretations concerning the "XCN" band in interstellar ice analogues (Hudson & Moore 2000); Carbonic acid production in H_2O:CO_2 ices. UV photolysis vs. proton bombardment (Gerakines et al. 2000); ROCN Species Produced by Ion Irradiation of Ice Mixtures: Comparison with Astronomical Observations (Palumbo et al. 2000); Hydrogen Isotopic Substitution Studies of the 2165 Wavenumber (4.62 Micron) "XCN" Feature Produced by Ion Bombardment (Palumbo et al. 2000); Chemically driven desorption of CO from icy grains in dark clouds (Takahashi & Williams 2000); Laboratory and astronomical IR spectra: an experimental clue for their comparison (Baratta et al. 2000); Solid-State CO toward rho Ophiuchi Elias 25: Ice Thresholds Revisited (Shuping et al. 2000); ISO-SWS observations of interstellar solid 13CO2: heated ice and the Galactic 12C/13C abundance ratio (Boogert et al. 2000); Ab Initio Quantum Chemical Studies of Reactions in Astrophysical Ices. 1. Aminolysis, Hydrolysis, and Polymerization in H_2CO/NH_3/H_2O Ices (Woon 1999); Ices and extinction through the Taurus and Ophiuchus clouds (Teixeira & Emerson 1999); Discovery of solid HDO in grain mantles (Teixera et al. 1999); Laboratory studies of thermally processed H_2O-CH_3OH-CO_2 ice mixtures and their astrophysical implications (Ehrenfreund et al. 1999); Measurements of the 44 μm band of H_2O ice deposited on amorphous carbon and amorphous silicate substrates (Maldoni et al. 1999); Laboratory Studies of the Formation of Methanol and Other Organic Molecules by Water+Carbon Monoxide Radiolysis: Relevance to Comets, Icy Satellites, and Interstellar Ices (Hudson & Moore 1999); The infrared band strengths of CH_3OH, NH_3 and CH_4 in laboratory simulations of astrophysical ice mixtures (Kerkhof et al. 1999); New 3 Micron Spectra of Young Stellar Objects with H_2O Ice Bands (Brooke et al. 2000); Weak ice absorption features at 7.24 and 7.41 micron in the spectrum of the

obscured young stellar object W33A (Schutte et al. 1999); The Interstellar 4.62 Micron Band (Pendleton et al. 1999); Methanol: The second most abundant ice species towards the high-mass protostars RAFGL7009S and W33A (Dartois et al. 1999); UV Irradiation of Polycyclic Aromatic Hydrocarbons in Ices: Production of Alcohols, Quinones, and Ethers (Bernstein et al. 1999); Observations of Solid Carbon Dioxide in Molecular Clouds with the Infrared Space Observatory (Gerakines et al. 1999); Constraints on the abundance of solid O_2 in dense clouds from ISO-SWS and ground-based observations (Vandenbussche et al. 1999); Carbon dioxide-methanol intermolecular complexes in interstellar grain mantles (Dartois et al. 1999).

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Identification of molecular-cloud material in interplanetary dust particles (Messenger 2000); Aromatic Moieties in Meteorites: Relics of Interstellar Grain Processes? (Sephton & Gilmour 2000); Infrared spectra of meteoritic SiC grains (Andersen et al. 1999); The SIC Problem: Astronomical and Meteoritic Evidence (Speck et al. 1999); Spectroscopic Evidence for Interstellar Grain Clumps in Meteoritic Inclusions (Sakata et al. 1999); Porous interstellar grains; A Singular Presolar SIC Grain with Extreme ^{29}Si and ^{30}Si Excesses (Amari et al. 1999), An infrared spectral match between GEMS and interstellar grains (Bradley et al. 1999).

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Distribution and Evolution of CH4, N2, and CO Ices on Pluto's Surface: 1995 to 1998 (Grundy & Buie 2001); Solar Gardening and the Seasonal Evolution of Nitrogen Ice on Triton and Pluto (Grundy & Stansberry 2000); The Effect of Methanol Clathrate-Hydrate Formation and Other Gas-Trapping Mechanisms on the Structure and Dynamics of Cometary Ices (Notesco & Bar-Nun 2001); Water Ice on Triton (Cruickshank et al. 2000); A detection of water ice on Jupiter with Voyager IRIS (Simon-Miller et al. 2000); Note: IR spectra of irradiated cometary ice analogues containing methanol: A new assignment, a reassignment, and a nonassignment (Hudson & Moore 2000); IR Detection of H2O2 at 80 K in Ion-Irradiated Laboratory Ices Relevant to Europa (Moore & Hudson 2000); Water Ice in 2060 Chiron and Its Implications for Centaurs and Kuiper Belt Objects (Luu et al. 2000); Evidence for Crystalline Water and Ammonia Ices on Pluto's Satellite Charon (Brown & Calvin 2000); NOTE: an Experimental Study of the Isotopic Enrichment in Ar, Kr, and Xe When Trapped in Water Ice (Notesco et al. 1999); Near-Infrared Spectra of Icy Outer Solar System Surfaces: Remote Determination of H2O Ice Temperatures (Grundy et al. 1999); Composition, Physical State, and Distribution of Ices at the Surface of Triton (Quirico et al. 1999); NOTE: Detection of Water Ice on Saturn's Satellite Phoebe (Owen et al. 1999); Evidence for Methane Segregation at the Surface of Pluto (Douté et al. 1999).

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