

COMMISSION 14: ATOMIC AND MOLECULAR DATA

(DONNEES ATOMIQUES ET MOLECULAIRES)

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As a result of the deliberations and discussions during the last General Assembly of the IAU in The Hague, it was recommended that Commission 14 become a commission of the Executive Committee. The special interdisciplinary role and nature of Comm. 14 were in this way recognized and encouraged.

Comm. 14 fulfills its role by informing the astronomical community of new developments in our various fields through specific involvement and support of IAU Symposia and Joint Discussions, and by the Reports of the Working Groups. The symposia and JDs are especially important means by which we acquire and provide information on the needs for, and availability of, atomic and molecular data. The most recent such example, co-supported by Comm. 14, was IAU Symposium 178, *Molecules in Astrophysics: Probes & Processes*, July 1-5, 1996, Leiden, The Netherlands. During the IAU General Assembly in Kyoto, Japan, August 18-30, 1997, Comm. 14 will co-support Symposium 188, *The Hot Universe*; JD4, *Challenges in Atomic Physics for Cosmic X-Ray Spectroscopy*; JD16, *Spectroscopy with Large Telescopes on Chemical Peculiar Stars*; and JD12, *Electronic Publishing Now and the Future*.

The reports from the Working Groups appear below where the highlights and triennial references of activities are given. The reference lists always have added value because of the expert selectivity of WG Chairs. For these triennial reports, the scope of the references have been expanded by the Chairs to include URLs of databases for atomic and molecular data. In order to make the WG reports more generally accessible, we have made them available on-line from the Comm. 14 WWW Home Page (<http://cfa-www.harvard.edu/amp/iau14/>).

We express very best wishes and encouragement to Dr. Jean Gallagher and I thank Dr. Dave Schultz for preparing and writing, with little notice, the WG3 report.

WORKING GROUP 1: ATOMIC SPECTRA AND WAVELENGTHS STANDARDS

W. C. Martin, Chair

The references cited for all categories of data in this report comprise a supplement for the period 1993–1996 to two previous reports: (1) the 1994 report of this working group covering the period 1991–1993, and (2) an extensive review of atomic spectroscopic data for astrophysics covering the literature to 1991 (Martin 1992).

Energy-Level Analyses, Wavelengths and Line Classifications

The references cited in this section are mostly papers on original laboratory research; recent larger compilations are covered in another section. The references, ordered by atomic number and spectrum, are given in parentheses following the spectra 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 this report.

Li I (R5); **Be** I (K1); [**N** II] (B5, S3), **N** VI (E2); **O** VII (E2); **Ne** I (C1), **Ne** II (Q1); **Al** X (K2); [**Si** I] (B8), **Si** III (S1), **Si** XI (K4, K2); [**P** II] (B6); [**S** I] (B9), **S** VIII (B1), **S** XIII (K2), **S** XV (H1); **Ar** II (P2, Q2), **Ar** IV (B4), **Ar** X (B2), **Ar** XV (K2); **K** II (V1); **Ca** III (V1); **Ti** XIII (J1); **Fe** I (N2, N3, J2, B7), **Fe** II (N1, B3), **Fe** III (E1), **Fe** VI (A1), **Fe** XXIV (R3); **Co** I (P1), **Co** VII (R6); **Ni** I (L2), **Ni** XXIV (M1); **Zr** III (R4); **Pd** II (L1); **Dy** III (S2); **Er** I (K3); **Pt** III (R1); **Au** II (R2), **Au** III (W2), **Au** IV (W1), **U** II (B10).

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/or stellar spectroscopy, especially for chemically peculiar stars. The references for the lighter elements are also incomplete, the selection being limited to those of highest astrophysical interest. The data in a number of the references include and/or supersede all or most of the previously available energy-level and wavelength data for the indicated spectrum; such references include those for **Be** I (a compilation), **Si** XI (K1), **S** VIII, **Ar** IV, **Ti** III, **Fe** I (N2), **Fe** XXIV, **Co** I, **Ni** I, **Dy** III, **Pt** III, and **Au** II. In a paper not cited above, Kelly and Lacy (1995) give accurate wavenumbers for fine-structure transitions in nine spectra ([**Ne** V] to [**Fe** II]) as determined from astronomical observations in the mid-infrared region. With regard to the iron-group elements, laboratory work is now underway on **Ti** II, **V** I, **Cr** III, **Mn** II, **Fe** II, **Fe** III, **Fe** V, **Fe** VI, and **Co** II; much of this research is being carried out at the University of Lund, Sweden, with additional work at Imperial College, London (**Fe** III and **Co** II), the Universities of Liège and Mons-Hainaut (**V** I), and the Observatoire de Paris (**Mn** II).

Wavelength Standards

Nave *et al.* (1996) have determined very high-accuracy Ritz wavelengths for 473 vacuum-ultraviolet **Fe** II lines (927–1995 Å). They recommend the new values as standards, the uncertainties lying mainly in the range 0.0001 to 0.0003 Å. These new **Fe** II standards, like several sets of high-accuracy wavelength determinations cited in our previous reports, depend on visible-region **Ar** II reference standards from Norlén (1973). New measurements of the **Ar** spectrum from a hollow-cathode discharge by Whaling *et al.* (1995) give **Ar** II wavenumbers systematically greater than Norlén's values by about 7 parts in 10^8 ; adjustment of the new **Fe** II results of Nave *et al.* to the **Ar** II wavenumber values of Whaling *et al.* would decrease the **Fe** II wavelengths by 0.00006 to 0.00014 Å.

The paper by Whaling *et al.* gives high-precision Ritz wavelengths for hundreds of **Ar** II lines over the range 2225 Å to 5.33 μm. The wavenumber uncertainties of most of the lines are less than 0.001 cm^{-1} , but the values are uncorrected for any pressure shifts. A number of the lines in the range 3600 Å to 3.27 μm are indicated as especially appropriate for use as reference standards because of their small pressure shifts. The systematic disagreement of 7 parts in 10^8 between these **Ar** II wavenumber determinations and those by Norlén "is roughly twice the uncertainty assigned to the wavenumbers in either experiment" (Whaling *et al.* 1995). The indicated need for additional measurements is, according to Nave *et al.*, being met by experiments underway in other laboratories.

Larger Compilations, Reviews, Conference Proceedings

The atomic data for absorption lines compiled by Verner *et al.* (1994) include data for 2249 lines having wavelengths greater than 228 Å. Shirai *et al.* (1996b) have completed a large single-volume tabulation of spectral-line data for highly-ionized atoms of **Ti** through **Cu**, and **Kr** and **Mo**. The energy levels of the **Zn** spectra (**Zn** I–XXX) have been compiled (Sugar and Musgrove, 1995), and a new compilation of data for the **Ga** spectra (**Ga** I–XXXI) includes classified lines and separate tables of energy levels (Shirai *et al.* 1996a).

The data in most of the newly published major compilations of these types are now also available via the Internet; for example, all of the above compilations except the absorption-line data are accessible at the NIST Physics Laboratory Web site, and the absorption data are included in the holdings of the "Atomic Data for Astrophysics" site (see below for the addresses of Web sites mentioned in this paragraph). It is also worth noting that some of the newly compiled or updated data being loaded into Internet databases may not be published in printed form. The energy-level data for the C, N, and O spectra in the NIST database for example, include some updating of the older compilations. Quite large datasets previously available only on magnetic tape or CD-ROM's have also been made available via the Internet, examples being the Kurucz CD-ROM 23 (CfA site, see Smith *et al.* 1996) and the "Atomic Spectral Line List" of R. Hirata and T. Horaguchi (CDS site, Catalogue VI/69). The "Vienna Atomic Line Data Base" is accessible only via e-mail (Piskunov *et al.* 1995).

A number of papers on atomic spectroscopic data are included in the proceedings of a workshop on *Laboratory and Astronomical High Resolution Spectra* (Sauval *et al.* 1995), and a few such papers were given at an IAU Joint Discussion on *Astrophysical Applications of Powerful New Databases* (Adelman and Wiese 1995). The invited papers given at the *Fifth International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas*, held in Meudon, France, August 1995, are scheduled for publication (Tchang-Brillet *et al.* 1996a). Many of the contributed papers for this colloquium were on particular spectra of astrophysical interest; these appear in a publication of the Paris Observatory (Tchang-Brillet *et al.* 1996b).

Atomic Spectroscopic Data on the Internet

The amount of atomic and molecular data conveniently available via the Internet has greatly increased very recently (since early 1995). 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.).

Unless otherwise indicated, the italicized names represent hypertext links that yield the data directly online. No detailed descriptions of the holdings or other features of the databases are given; since most of the databases are under development, even the *minimal information* provided here may in some cases be out of date by the time this report is published. The list includes only databases that offer one or more of the above three types of data and, even so, is not complete. A Weizmann Institute site (see below) maintains an updated hypertext 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. Links to new databases are added as they come online. 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.

CDS (Centre de Données astronomiques de Strasbourg, France)

<http://cds-web.u-strasbg.fr>

Select **Catalogues** and **VI Miscellaneous** (CL, EL, TP) and choose from a list of catalogues including several with extensive atomic spectroscopic data. Items from journals (*journal title*) include additional

catalogues with atomic spectroscopic data. Some catalogues are searchable (use *VizieR*), others accessible only via ftp. Select *TOPbase* (TP) and make a telnet connection to a database system incorporating data from the Opacity Project. Topbase data files can be transferred via ftp.

Astronomical Data Center (NASA Goddard Space Flight Center, U.S.A.)

<http://adc.gsfc.nasa.gov>

Select *ADC's Archives* (CL, EL, TP). Archives include extensive files of atomic spectroscopic data, having a large overlap with the CDS catalogues (see above) and other CDS holdings. Items of interest can be identified by online keyword searches, but data are accessible only via ftp. Site also has lists of contents of ADC CD-ROM's, one of which includes atomic spectroscopic data (CL, EL, TP).

WWW Server in NAOJ/ADAC (National Astronomical Observatory, Japan)

<http://adac.mtk.nao.ac.jp>

The *Clickable list of the catalogs* and *Miscellaneous Data* (CL, EL, TP) yield a list including the CDS catalogues (see above). Data are transferred via ftp.

NIST Physics Laboratory (National Institute of Standards and Technology, U.S.A)

<http://physics.nist.gov>

Select *Physical Reference Data* and *Atomic Spectroscopic Database* (CL, EL, TP), a component of the NASA Astrophysics Data System; also *Spectrum of Platinum Lamp* (CL) and *Bibliographic Database on Atomic Transition Probabilities*. Site has other atomic databases, and also molecular databases of astrophysical interest.

CfA Atomic and Molecular Physics Division (Harvard-Smithsonian Center for Astrophysics)

<http://cfa-www.harvard.edu/amp>

Select *Databases* and *Kurucz CD-ROM 18*, *Kurucz CD-ROM 23* (CL, TP) or *R. L. Kelly* (CL). Links to some other sites (Smith *et al.* 1996).

Atomic Data for Resonance Absorption Lines (Herzberg Inst. of Astrophysics, Canada)

http://www.dao.nrc.ca/~dcm/atomic_data.html

Select from several files (CL, TP) including finding lists (Morton 1991, with updating).

Atomic Data for Astrophysics (University of Kentucky, U.S.A)

<http://www.pa.uky.edu/~verner/atom.html>

Select *Energy Levels*, *Wavelengths*, *Transition Probabilities* (CL, TP). Data for resonance and absorption lines (Verner *et al.* 1994). Links to a number of other databases or datasets, mainly CDS catalogues.

SAM Project (NASA Goddard Space Flight Center, U.S.A.)

<http://aniara.gsfc.nasa.gov/sam.html>

Lists of Results (CL, TP) are sorted according to types of data, including calculated oscillator strengths. Some of the files are accessible via ftp only.

An atomic spectroscopic database being developed as a Web site at the University of Lund, Sweden, is expected to go online during 1997. The URL: <http://Rydberg.fysik.lu.se>.

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WORKING GROUP 2: ATOMIC TRANSITION PROBABILITIES

W. L. Wiese, Chair

The Data Center on Atomic Transition Probabilities at the National Institute of Standards and Technology (NIST) Gaithersburg, MD 20899, USA is continuing its critical data compilation work and is also participating in the development of a comprehensive atomic spectroscopic database of which a first version is installed on the World Wide Web. This database may be accessed from the NIST Physics

Laboratory WWW homepage at <http://physics.nist.gov/>. Further details on this and several other atomic spectroscopic databases on the Internet are given in the report of Working Group 1.

The comprehensive NIST bibliographical database, which now contains more than 6,600 entries, has been updated through June 1996 and is also available at the above cited World Wide Web site.

The current compilation work of the NIST atomic transition probabilities data center is centered on the evaluation and tabulation of numerical data for the lighter elements. Work is in progress on hydrogen, helium, lithium, beryllium, boron, fluorine, neon, sodium, and magnesium. The tabulations include allowed (electric dipole) as well as forbidden (mainly magnetic dipole and electric quadrupole) lines.

Some major works on transition probability and lifetime data during the last three years are the following:

- (a) In early 1996, the NIST data center published a 532-page volume of critically evaluated transition probabilities for the three elements carbon, nitrogen and oxygen as Monograph No. 7 of the Journal of Physical and Chemical Reference Data. This volume contains about 12,500 transitions for all 21 spectra of these three elements.
- (b) A large amount of data resulting from the Opacity Project and its successor, the Iron Project, has been published. For example, very extensive sophisticated calculations of transition probabilities for various ions of iron [4, 69, 75, 76, 78, 87] have been undertaken.
- (c) Systematic and accurate multi-configuration calculations of transition probability data have been undertaken by a group of theoreticians under the leadership of Froese Fischer, Hibbert, and Brage (members of the SAM-project). This group maintains a World Wide Web site (address: <http://aniara.gsfc.nasa.gov/sam/sam.html>) from which new results are available.
- (d) A large review concerned with data for lines starting from the ground states of many atoms and ions has been published by Verner et al. [102] Their listings contain 2,249 spectral lines, and the data are drawn mostly from the Opacity Project and recent critical compilations.
- (e) Another review of neutral line oscillator strengths has been published by Doidge [34]. This compendium contains oscillator strengths for neutral atomic resonance lines of 65 elements and has been collected mostly for the needs of laboratory atomic absorption spectroscopy.
- (f) A new edition of "Astrophysical Quantities" prepared by Cowley *et al.* [31], contains oscillator strength tables for about 500 prominent lines of astrophysical interest.
- (g) Finally, it is of interest to note that a number of informative review articles on the status and accuracy of oscillator strength data were given at the 5th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas, the proceedings of which are in preparation (see Tchang-Brillet [98]).

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 report left off. As in the previous reports, the bibliographical material is ordered with respect to element and state of ionization. Table 1 provides an overview of the bibliographical data by spectrum. The references are identified by a running number which refers to the general reference list at the end of this report. In the general reference list the literature is ordered alphabetically according to 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.
- CA - Coulomb approximation

EXPERIMENTAL METHODS:

- E - measurements in emission (arc, furnace, discharge tube, shock tube, etc.).
- A - measurements in absorption (King furnace, absorption tube, etc.).
- L - lifetime measurements (including Hanle effect).
- M - miscellaneous experimental methods (for example, Stark effect, astrophysical measurements, etc.).

OTHER:

CP - data compilation.

R - relative (non-absolute) been determined.

F - data on forbidden (i.e. other than electric dipole) transitions have been determined.

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TABLE 1. Important Literature References

Al I: 72	Cs I: 56, 96	O I: 106 O II: 106 O III: 46, 106 O IV: 106 O V: 41, 44, 106
Ar I: 49, 61 Ar II: 55, 80, 91 Ar III: 80	Fe I: 3, 37, 64 Fe II: 4, 8, 26, 36, 59, 75, 78, 87 Fe III: 76 Fe VIII: 69 Fe IX: 69 Fe X: 69, 101	P I: 13 P II: 45
B I: 27, 83 B II: 41, 50, 105, 108	Ga I: 66 Ga II: 43	Rb I: 67, 95
Ba I: 71 Ba II: 84	He I: 28, 29, 49, 65, 88, 104	S I: 14, 40 S II: 23, 61 S III: 53, 77, 97 S IV: 72 S V: 22
Be I: 105 Be III: 90	Hg II: 70, 90	Si: 77 Si II: 7, 25, 72
Bi I: 24	K I: 67	Sr I: 71 Sr II: 84
C I: 106 C II: 10, 39, 106 C III: 63, 106	Kr I: 49, 74, 92 Kr II: 16	Ti II: 15, 64
Ca I: 17, 19, 35 Ca II: 19, 57, 58	Li I: 17, 30, 67, 107	Tl II: 20 Tl III: 20
Cd II: 86 Cd III: 54	Mg I: 22 Mg II: 99 Mg III: 90	Xe I: 2, 74 Xe II: 9, 11, 21 Xe III: 11
Cl I: 12 Cl II: 58	N I: 100, 106 N II: 47, 106 N III: 5, 10, 38, 106 N IV: 42, 106	Zn I: 109 Zn II: 6, 90
Co I: 81 Co II: 32	Na I: 18, 67, 68, 82, 103 Na II: 51 Na III: 33	
Cr I: 89 Cr II: 6, 52, 85, 94	Nc I: 49, 62, 79 Nc II: 62 Nc III: 33	

WORKING GROUP 3: COLLISION PROCESSES

D. R. Schultz

Excitation and ionization of atoms and ions by electron-impact continues to be an area of very active investigation. Access to the most up-to-date data produced may be obtained either through new works which provide collections, evaluations, and recommendations, or through the original works which can be located through bibliographic databases and articles.

For example, a new collection of recommended cross sections for excitation and ionization of the ground and excited states of atomic hydrogen has been compiled by Janev and Smith [1] complementing earlier work which also included collisions with ground and excited hydrogen molecules, hydrogen molecular ions, helium, and helium ions [2]. Also, an extremely valuable and comprehensive work is contained in the proceedings and collected results of the atomic data assessment meeting hosted by the Rutherford Appleton Laboratory in 1992 [3]. This meeting was the latest in a series of meetings beginning in 1975 which have taken as their goal the elucidation of atomic data for astrophysical and laboratory plasmas. The present volume [3] provides collections of references, compilations of cross sections and rate coefficients, and some recommended values for these, for atoms and ions ranging H to Fe.

Other reviews and collections of electron-impact data appearing during the period 1993-1996 include a compilation of data for important nebula emission lines by Pradhan and Peng [4] and a review of excitation of C, O, Fe, and rare gas ions by Tayal *et al.* [5]. The latter is part of a compendium [6] also containing reviews and recommendations of data for elastic scattering, ionization, and recombination in low temperature fusion plasmas.

Large scale projects and ongoing lines of data generation by key producers also continue to increase the knowledge base of electron-impact phenomena. In particular, the so-called Iron Project has sought to bring together a number of experts to provide fine-structure collision strengths and rate coefficients for Fe ions and other ions of heavy elements, along the lines of the previous Opacity Project. Data from the Opacity Project (TOPbase) is directly available through the widely used *file transfer protocol (ftp)*. TOPbase is available at the Centre de Donnés de Strasbourg, France (at Internet Protocol (IP) address 130.79.128.5, with account name "topbase" and password "Seaton+") and NASA Goddard Space Flight Center (IP: 128.183.101.54, same account name and password). A brief description of the project, a list of important references, and instructions for downloading files may conveniently be found on the World Wide Web (at URL <http://astro.u-strasbg.fr/OP.html>). Work is underway to provide Web-based access to the Iron Project data (TIPbase, see URL <http://www.am.qub.ac.uk/projects/iron/>). This Web site also lists the papers in the Iron Project series (we repeat this list here for the reader's convenience [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]). A hyperlink can also be followed to a database containing electronic versions of the published articles. Current publications may also be accessed on-line in the *Astronomy and Astrophysics Supplement Series* (URL <http://www.ed-phys.fr/docinfos/OnlineAetA.html>).

Other recent published articles which represent continuations or extensions of work which seeks to compute electron-impact data for various iso-electronic or iso-nuclear sequences are represented by the relativistic distorted wave calculations of collision and oscillator strengths for $\Delta n = 0$ transitions in B-like ions by Zhang and Sampson [27, 28], cross sections and rate coefficients for excitation of $\Delta n = 0$ transitions in Be-like ions with $6 \leq Z \leq 54$ by Safronova *et al* [29], and the collision strength and radiative decay rate calculations of Bhatia and Doschek for Fe X [30], Ne V [31], Mg VII [32], and Si IX [33]. These recent papers were all published in *Atomic Data and Nuclear Data Tables*. Consequently, an important resource for locating electron-impact data is the cumulative index of this journal. This index along with the cumulative author index is distributed to subscribers and is now available on-line on the World Wide Web (URL <http://www-cfadc.phy.ornl.gov/adndt/adndt.html>).

In fact, atomic data are becoming much more accessible with the advent of on-line resources. For example, much of the data on electron-impact ionization of ions measured at the Oak Ridge National Laboratory Multicharged Ion Research Facility over the last twenty years are now available through the World Wide Web (URL <http://www-cfadc.phy.ornl.gov/xbeam/xbintro.html>) in both graphical and tabular form. Other resources on the Web include access to bibliographic databases. The Oak Ridge National Laboratory Controlled Fusion Atomic Data Center (CFADC) maintains an on-line database of references to atomic collision data containing approximately 29,000 articles dating from 1978 to present which have been categorized by reaction (URL <http://www-cfadc.phy.ornl.gov/search.html>). A completely independent bibliography searchable by reaction category is provided by the Laboratoire de Physique des Gaz et des Plasmas at the Universite Paris-Sud, Orsay, France (URL <http://gaphyor.lpgp.u-psud.fr/>). Annotated bibliographies are also available such as that for electron collisions with positive ions by Itikawa [34] and the *International Bulletin on Atomic and Molecular Data for Fusion* available from the International Atomic Energy Agency [35]. The content of the *Bulletin*, however, is largely composed from the updated files of the CFADC on-line bibliography, and therefore, the newly available World Wide Web sites will provide generally the most up-to-date and easily accessible source of bibliographic information.

It should be noted that significant progress has been made both theoretically and experimentally over the past three years in advancing the techniques of studying electron-impact phenomena. For instance, the use of ion-storage rings, which utilize electron-coolers, as platforms for electron-ion reactions, promises to provide new levels of detail in recombination, excitation, and ionization cross sections (see e.g. Kenntner *et al.* [36]). From a theoretical point of view, new techniques are being developed that have similarly advanced the state-of-the-art for few-electron systems such as the convergent close coupling method of Bray and Stelbovics [37], the hyperspherical close-coupling approach of Kato and Watanabe [38], the R-matrix with pseudo-states method of Bartschat *et al.* [39], the direct solution of the Schrödinger equation on a numerical lattice [40], and the extension of perturbation theory approaches through inclusion of improved approximations to the final state wavefunction [41, 42].

Finally, it is worth noting some statistics regarding the number of works published between 1993 and 1996 regarding electron-impact excitation and ionization. Using the CFADC on-line database, it is found that many works concentrate on the fundamental one and two-electron targets H and He (about 60 references regarding ionization in collisions of electrons with H, He⁺, and He, and about 75 regarding excitation in these systems). In contrast, only about 25 references were found to ionization of all ions of Li, Be, B, C, N, and O, (about 30 regarding excitation). Interest is also focused on certain challenging and key species such as iron ions (15 references for ionization, about 40 for excitation). Clearly, the continued study of electron-impact of atoms and ions will further the refinement of cross sections, rates, and strengths for systems already studied, and provide new information for those which remain unexplored.

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CHEMICAL REACTIONS

The following table of measurements of reaction rates at low temperatures was provided to W. H. Parkinson by Ewine F. van Dishoeck.

TABLE 2. Neutral Reactions Studied at $T \leq 295$ K in Birmingham/Rennes

Reaction	T range	Type	Reference
CN + O ₂	99-761 K	cell	Sims & Smith 1988, Chem. Phys. Lett. 151 , 481.
CN + NO + M	99-450 K	cell	Sims & Smith 1993, J. Chem. Soc. Faraday Trans. 89 , 1.
OH + HCl, C ₂ H ₆ OH + CH ₄	138-298 K 178-298 K	cell	Sharkey & Smith 1993, J. Chem. Soc. Faraday Trans. 89 , 631.
OH + CO	80-298 K	cell	Frost <i>et al.</i> 1993, J. Phys. Chem. 97 , 12,254.
CN + O ₂ CN + NH ₃	13-295 K 25-295 K	CRESU	Sims <i>et al.</i> 1994, J. Chem. Phys. 100 , 4,229.
CN + C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ CN + CH ₄ , C ₃ H ₆	25-298 K 160-298 K	combined cell	Sims <i>et al.</i> 1993, Chem. Phys. Lett. 211 , 461.
OH + N OH + O	103-294 K 158-294 K	cell	Smith & Stewart 1994, J. Chem. Soc. Faraday Trans. 90 , 3,221.
OH + but-1-ene, (E- & Z-) but-2-ene	23-295 K	CRESU	Sims <i>et al.</i> 1994, J. Chem. Soc. Faraday Trans. 90 , 1,473.
OH + HBr	23-295 K	CRESU + theoretical	Sims <i>et al.</i> 1994, J. Chem. Phys. 101 , 1,748.
OH + NO + M	23-301 K	combined	Sharkey <i>et al.</i> 1994, J. Chem. Soc. Faraday Trans. 90 , 3,609.
NO(X ² H) rovibrational energy transfer	80-295 K	cell	Islam <i>et al.</i> 1994, J. Phys. Chem. 98 , 9,285. Islam <i>et al.</i> 1995, J. Chem. Phys. 103 , 9,676.
CH + O ₂ , NO CH + NH ₃	13-708 K 23-295 K	combined CRESU	Bocherel <i>et al.</i> 1996, J. Phys. Chem. 100 , 3,063.
CH + N	216-584 K	cell	Brownsword <i>et al.</i> 1996, J. Chem. Soc. Faraday Trans. 92 , 723.
CH(v=1) + CO, N ₂	23-584 K	combined	Herbert <i>et al.</i> , J. Phys. Chem., submitted.
CH + CH ₄ , C ₂ H ₂ , C ₂ H ₄ C ₂ H ₆ and but-1-ene	23-295 K	CRESU	Canosa <i>et al.</i> , A & A, submitted.
CH + H ₂ → CH ₃ by radiative assn.		theoretical	Brownsword <i>et al.</i> , ApJ, in preparation.
CH(v=0,1) + H ₂ , D ₂	13-744 K	combined	Brownsword <i>et al.</i> , J. Chem. Phys., in preparation.

WORKING GROUP 4: LINE BROADENING

N. Feautrier, Chair

The field of line broadening has continued to be very active during the last three years, as could be observed during both the 12th International Conference on Spectral Line Shapes (ICSLS, Toronto 1994) (1) and the 13th ICSLS (Firenze 1996) (2). This activity has been mostly stimulated by the interpretation of recent observations or by the preparation of space investigations.

During the last period, most of the works were concentrated on applications of methods established in the preceding years, yielding many results, so new data bases were elaborated and existing ones improved. It is not the aim of this report to be exhaustive; we will simply give a selection of references on the basis of their astrophysical interest.

Stark Broadening**STARK BROADENING FOR PLASMAS OF LOW DENSITIES: THE IMPACT LIMIT**

For diffuse to moderately dense plasmas, the Opacity Project includes extensive calculations of atomic data required for opacity determination, particularly Stark broadening constants for atomic and ionic lines involving relatively low excited states. These data are very precise, and approximate formula are available for transitions involving higher excited states.

Approximative methods (\bar{g} method, semiclassical perturbative theory) have been used extensively to provide broadening parameters with a mean accuracy better than 30 percent for a large number of lines. Some results are only available in electronic form via an anonymous ftp to the CDS center (see the Editorial in A&AS, Vol. 103, No1). Furthermore, much work of high quality has been done experimentally.

Table 3 presents results for many transitions; the numbers refer to the reference list.

TABLE 3. Important Literature References

Al I, III, XI	3, 4, 5	Na I, IV	20, 21
Ar II	6, 7	Ne VII, VIII	22, 21
AsII	8	Ni I, II	23,24
B I	9	N V	13
Be I	10	O IV, V, VI	25, 26, 13
Bi II	11	Pa I	27
Br II	8	S III, IV	28
C II, IV	12, 13	Sb II, III	6
Ca II	14	Si XII	5
Cd II	15	V I	29
Fe II, VII	16, 17, 18	Zn II	15
Mg I	19		

Results for isoelectronic sequences, such as B-sequence (9), or series four and five times charged ion lines (30) are of particular interest. Because of the speed with which such calculations can be made, it would be interesting that more systematic work be done and presented as a data base. A complementary *direction concerns investigations of systematic trends of Stark broadening parameters. Regularities of these parameters have been investigated (31). Finally, one should mention an important work on the Stark broadening theory of solar Rydberg lines (32, 33) and an interesting study of the profile of the Pa line of H from the line center to the far wings under the physical conditions of stellar atmospheres (34).*

BEYOND THE QUASISTATIC LIMIT FOR IONIC PERTURBERS: HOT AND DENSE PLASMAS AND/OR HYDROGENIC EMITTER

In the case of dense and hot plasmas, interactions with ionic perturbers become a major source of broadening. Due to the linear Stark effect, it is the same situation whether the emitter is an H atom or an hydrogenic ion. The quasistatic approximation used for ionic broadening at low densities is no longer valid and simultaneous strong interactions between the radiator and the surrounding perturbers must be taken into account. Much effort has been devoted to this many body dynamical problem both on the methods and the applications. Important results have been obtained theoretically or experimentally for lines of H (35-37), He⁺ (36, 38, 39), N V (40) and multicharged hydrogenic ions (41). Extensive tables (42) and parametrized formulae (43) are available. Analytic expressions have been obtained for the lines of one electron ions (44), and wing formulae for plasma broadened spectral lines of hydrogenic ions (45). Ion dynamics effects are also studied in He lines (46-49).

Far wings of the Lyman α line of H have been studied in a quasi molecular approach in the physical conditions of white dwarfs (50).

Line Broadening by Foreign Gases and Molecular Line Broadening

BROADENING OF ATOMIC LINES

Calculations involving various degrees of sophistication in the determination of interatomic interactions have been published: self broadening of He triplet lines (51), and Sr resonance line perturbed by H (52). One has to mention interesting results on the collisional broadening of Mg Rydberg lines (53) and of s-p and p-s atomic transitions of Na, Ca, and Fe (54) perturbed by H atoms.

MOLECULAR BROADENING

Many important results have been obtained, mainly in the infrared spectra. For astrophysical applications we will quote particularly the calculation of the broadening parameters of CO perturbed by He (55), and the self-broadening of N₂ (56). Many theoretical or experimental investigations in this domain have been stimulated by new spatial observations of planetary atmospheres or by the need of new molecular data in particular for Jupiter and Titan atmospheres. Particular attention has been paid to collisional broadening in various bands of CO₂ (55, 57), NH₃ (58-60), CH₄ (61-68), C₂H₂ (69), C₂H₄ (70), H₂O (71). A special attention has been paid to the problem of line mixing in CO (55), CO₂ (55), C₂H₂ (69). This considerable effort in molecular line broadening has contributed to improve molecular databases.

COLLISION INDUCED SPECTRA

Collision induced spectra contribute to a major part of the opacity in the outer planets, which are composed of non-polar species like H₂, and He. Recently a new interest for collision induced spectra has appeared with the need of opacities for the modelling of cool and dense stars: white dwarfs, brown dwarfs, etc.

Accurate calculations of H₂-H₂ (72), H₂-He (73), CO₂-CO₂ (74), N₂-N₂ (75), and CH₄-H₂ (69) pairs have been carried out. The accuracy of the results depends directly on the quality of the intermolecular potentials.

DATA BASES

A number of interesting papers have been published in the special issue of JQSRT (52, 1994) devoted to atmospheric spectroscopy applications. One has to mention in particular the Smithsonian Astrophysical Observatory Database which combines the best currently available line parameters (76), a PC/AT new version of Geisa Data bank (77), and the TDS spectroscopic databank for spherical tops like CH₄, CF₄, etc. (78).

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WORKING GROUP 5: MOLECULAR STRUCTURE AND TRANSITION DATA

E. F. van Dishoeck, Chair

The most significant development in the last three years has been the enormous expansion and availability of atomic and molecular databases in electronic form (CD-ROM, ftp, World-Wide-Web).¹⁻⁵ Millions of molecular lines ranging from the millimeter to the extreme ultraviolet part of the spectrum can now be accessed on-line, and improved software allows rapid searches through the data bases. At the same time, the astrophysical needs for such large data bases have increased considerably. Spectral line surveys at submillimeter wavelengths typically contain thousands of rotational lines,⁶ high resolution infrared spectra from the ground and the *Infrared Space Observatory* require large amounts of information on the vibrational transitions,^{7,8} whereas large format CCDs in the optical and ultraviolet allow large wavelength ranges to be scanned for electronic transitions. The astrophysical modeling has improved to the stage that highly accurate molecular data are essential. A well-known example, which has been studied intensively by several groups over the last decade, is provided by the VUV electronic transitions of CO.^{21,31} For models of cool stars and brown dwarfs, information on the weaker transitions, whose intensities are five orders of magnitude less than those of the strongest transitions, proves to be essential.⁹

There have been significant developments in the experimental techniques and theoretical methods for determining molecular structure, both of stable species, and of radicals and ions. Of particular interest is the progress in measuring and calculating the spectra of large molecules, including PAH's, long carbon chains and C₆₀.

The following summary is based on contributions sent to me by U.G. Jørgenson, T. Oka, J.P. Phillips, F. Rostas, P.L. Smith, and P. Thaddeus in the summer of 1996. Other topics have been added through a literature search. This report focuses on the highlights, and concerns only molecules of astrophysical interest. No attempt has been made to provide a complete overview or list of references. For further information on a specific molecule, the bi-monthly *Berkeley Newsletter* continues to be a good starting point. The

printed Newsletter is essentially a bibliography of articles in the current journals on molecules comprising four or fewer atoms (contact jphillips@astro.berkeley.edu or spdavis@physics.berkeley.edu).

Electronic spectra

The laboratory astrophysics group at the CfA has continued to provide quantitative, high spectral resolution measurements of molecules of atmospheric and astrophysical interest in the ultraviolet. Theoretical studies of the predissociation of the Schumann-Runge (S-R) bands of O₂ have been carried out for both rotational¹⁰ and isotopic dependency.¹¹ Absorption bands of the S-R system have been observed at 670 K at high resolution, and precise wavelength measurements have led to the molecular constants of the ground state of O₂.¹² Two highly excited ³II states of O₂ have been identified in collaboration with colleagues at the Photon Factory, Japan, and NRC, Canada.¹³ Absorption measurements at Doppler limited resolution have been carried out by Yoshino and colleagues with a VUV Fourier transform spectrometer (FTS) in combination with a White cell at Imperial College (IC), London, U.K. The O₂ Herzberg I band system ($A\ ^3\Sigma_u^+ - X\ ^3\Sigma_g^-$) has been measured at a resolution of 0.06 cm⁻¹;¹⁴ band oscillator strengths and rotational line strengths have been obtained.¹⁵ These are the first absorption intensity measurements of the Herzberg bands free of problems arising from inadequate spectral resolution. In addition, the NO $\delta(0,0)$ and $\beta(7,0)$ bands have been measured at a resolution 0.06 cm⁻¹ with the VUV FTS at IC.¹⁶ To extend the high resolution measurements to shorter wavelengths, the CfA/IC group moved this apparatus to the Photon Factory, Japan, where VUV radiation from a synchrotron source with a narrow band predisperser is available.¹⁷ Analysis of the measurements of the NO bands and the S-R bands of O₂ obtained with this facility are in progress. The absorption cross sections for the VUV diffuse bands of CO₂¹⁸ and H₂O¹⁹ have been measured.

The VUV spectrum of CO continues to be intensively studied by several groups. The CfA group has obtained photoabsorption cross sections of CO in the wavelength region 92.5 nm to 97.4 nm at ~20 K, thus greatly simplifying their application to astrophysical models.²⁰ The band oscillator strengths of the $A(v') - X(0)$ fourth positive bands of CO for $v' = 11 - 14$ have been obtained with high resolution²¹ and have confirmed the values of Chan et al.²² The Meudon group has also studied the $A^1\Pi - X^1\Sigma^+$ transition for ¹²C¹⁸O and ¹³C¹⁸O.^{23,24} Using the A state term values a new set of term levels for the B, C and E states has been established.²⁵

A new triplet state of CO (^k3II) has been analyzed through its interactions with the E and B states and by direct absorption measurements.^{26,27,28} The B¹Σ⁺ ($v=3$) level situated above the B¹Σ⁺-D'¹Σ⁺ crossing has been observed and calculated with the semi-empirical potentials established earlier.²⁹ A pulsed jet has been used in conjunction with the 10m vacuum spectrograph and the BRV pulsed continuum to obtain cooled spectra of the CO Rydberg states.³⁰

Predissociative and radiative lifetimes of the excited states of CO have been determined from line broadening measurements on singly resolved rotational states using a coherent and tunable VUV source by Ubachs and co-workers.^{31,32,33} For several states, the predissociation rates were found to depend on rotational state, parity and isotope. The E¹Π $v=0$ and 1 levels were carefully studied for ¹²CO and ¹³CO and were found to be strongly predissociated by the ^k3II bound state. The lifetime of the (4pπ)L¹Π $v = 0$ state (f parity) was determined at 1.0 ns, typical of a radiative rather than a predissociative lifetime.

Basic spectroscopic work on the most important astrophysical molecule, H₂, continues by the Meudon group. The photographic atlas of the Lyman and Werner bands has been published.³⁴ More than 12000 lines are tabulated, 96% of which have at least one assignment. New calculations concerning the B' and D states have been published.³⁵ Together with previous work concerning the B and C, states these allow precise calculations of the Werner and Lyman bands. Comprehensive tables of line positions and intensities are now available.^{36,37}

A new set of molecular constants for the ground state of N_2 has been established using all the data available in the different spectral ranges.³⁸ A comprehensive model of the first seven singlet Rydberg and valence states has been established. This will allow precise modeling of the VUV emission of N_2 in the atmosphere of Titan and the Earth around 100 nm.³⁹ The nf Rydberg levels of $^{14}N_2$ converging on the $X^2\Sigma_g^+$ state of N_2^+ have been studied.⁴⁰

Studies of the N_2^+ molecular ion have been made by the Berkeley group with a Pointolite arc which produces highly excited levels of the ion, and with a cooled hollow cathode lamp. The analysis was extended to much higher rotational energies as compared to the hollow cathode or furnace spectra.⁴¹ Bernath and co-workers used the Fourier Transform technique to study the electronic spectra of a number of astrophysically relevant molecules including CoH⁴⁵, CH⁴⁶ and the Swan system of C_2 .⁴⁷

Extensive electronic structure calculations continue to provide valuable information on potential energy surfaces, transition moments, spectroscopic constants and line intensities. A theoretical study of the NO ϵ , the 11000 Å, and the $b^4\Sigma^-$ bands has been made by the NASA-Ames group^{42,43,44}, who also computed the electronic states of MgC.⁴⁹ The ground and excited states of SiH⁺¹⁵² and CP¹⁵³ have been calculated by the Wuppertal group. Potential surfaces and line intensities of Si₂C⁴⁸, N_3^+ ,⁵⁰ NH₂⁺,⁵¹ and CO₂⁵² have been investigated theoretically by the French group. The flat shape of the N_3^+ $X^3\Sigma_g^-$ ground state along the asymmetric displacement coordinate leads to strong anharmonic resonances. For NH₂⁺, the quasilinear ground state and the bent quasi-linear $a^1A_1 - b^1B_1$ Renner-Teller system have been studied up to high energies. An exhaustive study of the excited electronic states of CO₂ suggests that the observed peculiar splittings of the first dipole-allowed electronic transition $1^1\Sigma_u^+ - X^1\Sigma_g^+$ are due to complex avoided crossings and vibronic coupling effects between the Rydberg and valence $1^1\Sigma_u^+$ states.

The Leiden group has performed comprehensive theoretical calculations of the absorption spectra of the lowest 10 electronic states of CH₂ and its isotopes.⁵³⁻⁵⁷ Similar work on NH₂ is in progress.⁵⁸ The HCO⁺ ion appears to be remarkably transparent to ultraviolet radiation, since all its dipole-allowed transitions lie at very high energies.^{59,60}

The transition rates for ZrO have been measured from a laboratory absorption spectrum by the Berkeley group, for the purpose of resolving differences between an earlier analysis of an emission spectrum, and experimental results and theoretical treatments.⁶¹ The spectrum of LaS from a carbon tube furnace has been produced and analyzed.⁶² A major theoretical effort by Langhoff on the gf values for all absorption lines of low-lying electronic states of TiO that would contribute to the opacity of cool evolved stars has just been finished.^{63,64}

The SCAN data base by Jørgenson⁹ contains information about the identification, frequency, excitation energy and strength of ~70 million lines from the molecules CN, CH⁶⁵, TiO, H₂O, HCN, C₂H₂ and C₃. The Harvard-Smithsonian data base on TiO, C₂, SiO, CN, CO, H₂, CH, NH, OH, MgH and SiH was recently reviewed by Kurucz.⁶⁶

There has been major progress in experimental and theoretical studies of larger molecules. The photofragmentation of model PAH monocations such as deuterated naphthalene⁶⁷ and benzene⁶⁸ has been studied using synchrotron radiation in the range 15-35 eV. The effect of molecular size has been evaluated.⁶⁹ The single and double ionization potentials of PAH's have been modeled by an empirical expression.⁷⁰ The formation, relaxation and destruction of negative PAH ions has been studied by an electron diffusion technique.⁷¹ The formation of PAH's in stellar envelopes has been modeled on the basis of the laboratory data. Small PAH's appear to be formed near the star and destroyed further out. Larger ones are formed at larger distances by condensation of the small PAH's produced initially.^{72,73} Ab initio studies of the electronic absorption spectra of some PAH cations have been made in the Bonn group.⁵⁷

The possibility that linear carbon chains are responsible for some of the diffuse interstellar bands has received renewed attention.^{74,75} Detailed absorption spectra of these chains and their cations in neon matrices have been obtained by Maier and co-workers.^{76–82} A possible assignment of two diffuse interstellar bands observed at near-infrared wavelengths with C_{60}^+ was made by Foing & Ehrenfreund,⁸³ based on spectra by Fulara et al.⁸⁴ The electronic spectroscopy of C_{60} has been studied in the Meudon laboratory between 200 and 750 nm by electron energy loss spectroscopy.^{85,70} Rotational band contours of C_{60} and linear carbon chains have been calculated and compared to the diffuse interstellar bands.⁸⁶ It is concluded that most DIB's would be due to molecules containing more than 10 atoms provided the excited states are coupled with isoenergetic vibronic levels of lower electronic states.

Vibrational spectra

The vibrational transitions of H_3^+ continue to be a popular topic among infrared spectroscopists. A highlight is the definite detection of interstellar H_3^+ by Geballe & Oka in absorption in the direction of deeply embedded protostars.⁸⁷ H_3^+ infrared emission lines were also detected in polar regions of Saturn. The lines are weaker than those in Jupiter by two orders of magnitude reflecting the lower plasma activity.⁸⁸ On the spectroscopic side, Oka and co-workers have observed the near-infrared $3\nu_2$ overtone band of H_3^+ at $1.4\ \mu\text{m}$ using InGaAsP communication diode lasers.⁸⁹ Spectral lines and the distribution of H_3^+ in extremely high rotational levels have been studied for supplying data to astronomers.⁹⁰ New experiments and analysis of the H_3^+ vibration-rotation spectra were also made by the NRC group in Canada,⁹¹ and by Maier's group.⁹² Spin selection rules in plasma chemistry of ortho- and para- H_3^+ has been experimentally demonstrated.⁹³

Oka also reported on the infrared spectra of several other ions. The spectrum of N_2H^+ in highly-excited vibrational states up $10600\ \text{cm}^{-1}$ has been observed and analyzed⁹⁴, as has the $\nu_2 + \nu_3 - \nu_2$ hot band of NH_3^+ ⁹⁵ and the infrared spectrum of NH_2^+ .⁹⁶ The infrared spectrum of CH_3^+ involving high rotational levels has been observed and the rotational distribution studied.⁹⁷ The spectrum of $C_2H_3^+$ was measured using a hollow cathode discharge, and its chemistry analyzed.⁹⁸

The infrared work at the Herzberg Institute of Astrophysics has concentrated on the spectra of weakly-bonded complexes, including CO- N_2 ,⁹⁹ CO-He,¹⁰⁰ and the HD dimer.¹⁰¹ Fundamental infrared spectroscopy has been performed for the ν_3 band of C_3 isotopes,¹⁰² C_4 ,¹⁰³ CH_3NC ,¹⁰⁴ CH_3OH isotopes,^{105–107} C_2H_2 and isotopes,^{109,109} and C_3O_2 .¹¹⁰ High resolution wave-number standards for the infrared have been published.¹¹¹

Bernath and co-workers have used the Fourier transform method to measure the infrared spectra of a large number of stable and unstable species, including ND, PH,¹¹² hot H_2O ,¹¹³ HF,¹¹⁴ SiO,¹¹⁵ CS,¹¹⁶ and SH.¹¹⁷ Pure carbon molecules, including C_{60} and C_{70} have been discussed.^{118–120}

Theoretical calculations of ground state potential energy surfaces and dipole moments have been made for CO,¹²¹ MgO^+ ,¹²² NO,⁴⁵ SiO,¹²³ and $C_2H_2^+$.¹²⁴ Theoretical infrared spectra for PAH's (neutral, cations and anions) have been computed by Langhoff.¹²⁵

Rotational spectra

Thaddeus has reported six new carbon chains detected in the laboratory, all of astrophysical interest: C_7H ,¹²⁶ C_8H ,¹²⁷ C_9H ,¹²⁸ $C_{11}H$,¹²⁹ $HC_{11}N$,¹³⁰ and $HC_{13}N$.¹³¹ The microwave and millimeter wave frequencies of these molecules are now known to a fraction of $1\ \text{km s}^{-1}$ in radial velocity. $HC_{11}N$, which for 14 years has stood as the largest interstellar molecule, was unfortunately misidentified. The claimed lines in IRC+10216 and TMC-1 are some entirely different molecule — the actual lines of $HC_{11}N$ lie 0.13%

lower in frequency, and are so far undetected. However, C₈H has been identified in IRC+10216 on the basis of the laboratory data,¹²⁷ and it seems likely that some or all of the other chains on this list will be detected in the fairly near future. The CfA/Harvard group has also been involved in investigating other species, including N₂H⁺,¹³² C₄H,¹³³ C₃N,¹³⁴ and HC₃S.¹³⁵

The submillimeter spectra of Orion/KL⁶ and other so-called "hot core" objects require detailed spectroscopy of complex organic molecules up to high frequencies. De Lucia, Herbst and co-workers have studied the submillimeter spectra of CH₃OD,¹³⁶ CH₃CHCH₂,¹³⁷ C₂H₅CN,¹³⁸ trans- and gauche ethyl-alcohol,^{139,140} and DCOOCH₃.¹⁴¹ Spectra up to the terahertz region have been measured in the Cologne laboratory of SO,¹⁴² CN,¹⁴³ and CH₃OH,¹⁴⁴ and in Lille of NH₃.¹⁴⁶ The microwave spectra of the simplest amino acid, glycine, have recently been measured by Lovas' group¹⁴⁵ for both conformers, enabling new astronomical searches.

The Lille group has also measured millimeter spectra of HCOCN,¹⁴⁷ H₂SiO,¹⁴⁸ Si₂H₂,¹⁴⁹ C₂H₃⁺,¹⁵⁰ and NH₂.¹⁵¹

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WORKING GROUP 6: MOLECULAR REACTIONS ON SOLID SURFACES

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Since the last Report there has been considerable recognition of the astrophysical importance of interstellar, interplanetary, and cometary dust and their function as sources of cosmochemical reactions. Laboratory studies and simulations, as well as increasing observation of interstellar, interplanetary and cometary materials have developed in number and in depth. It is noticeable that this area has become attractive to surface science scientists as evidenced by their participation in recent workshops and meetings. However, so far, in spite of their relevance to astrophysical problems, relatively few laboratory studies have been directed towards the chemical aspects of those molecular reactions on solid surfaces. This report therefore deals mainly with physical and physico-chemical properties of materials within this context. As was the last, the present report is non-exhaustive and seeks to give indications to key studies in this area. Basic references to surface science studies and techniques were given in the last Report.

Reviews and Meetings

- (i) Physical and Chemical processes in Icy Grain Mantles [Schmitt, B.: 1994, *Molecules and Grains in Space*: AIP Conf. Proc. **312**, 735].
- (ii) Nenner, I. (ed.): 1994, *Molecules and Grains in Space*: AIP Conf. Proc. **312**, pp.1-863.
- (iii) Millar, T.J. and Williams, D.A.(eds.): 1993, *Dust and Chemistry in Astronomy*, (IOP, Bristol).
- (iv) Cosmic Chemistry: Molecules in Space, Williams, D.A.: 1994, *Contemporary Physics* **35**, 269-283.
- (v) Circumstellar Matter. Watt, G.D. and Williams, P.M. (eds.): 1995, *Circumstellar Matter*, (Kluwer, Dordrecht).
- (vi) Shocks in Astrophysics. Millar, T.J. and Raga, A.C. (eds.): 1995, *Shocks in Astrophysics*, (Kluwer, Dordrecht).
- (vii) International Conference on Dust, Molecules and Backgrounds: From Laboratory to Space, 1995 (October issue), *Planet. Space. Sci.* **43**.

Studies of Dust Grain Properties and Models

Composition and radiative properties of grains in molecular clouds and accretion disks [85]; dust destruction mechanisms [19]; dust temperatures [103]; size distribution of dust particles [52]; modelling of processes from molecules to grains [101]; dust opacity and condensation models [39]; grain alignment processes in dark clouds [32, 114]; nova dust evolution and formation of HAC emission features [27]; formation of complex molecules on grain surfaces [42, 75]; chemical models involving gas-grain interactions [8, 37]; grains and shocks [28, 29].

Astrophysical Observations

Observations of hot amorphous carbon grains [119]; observations of high galactic latitude dust [50, 87, 104]; silicate cosmic dust observations and analogues [45, 54, 105]; possible detection of solid formaldehyde in the interstellar medium [100]; solid CO in Taurus Dark Cloud [18].

Laboratory Studies and Astrophysical Modelling of Carbonaceous Materials

Formation of carbon-based grains in the outflows of Red Giants: modelling [1, 2, 13, 17, 34]; photoelectric heating mechanisms of very small graphitic grains and polycyclic aromatic hydrocarbons (PAHs) [5]; coal model for the UV-visible interstellar extinction curve [36, 80-82]; laboratory spectra of PAH molecules and ions and the extinction curve [58, 59, 92, 93]; origins of variation of the 2175Å band in the interstellar extinction curve [64]; laboratory studies of carbon particles and clusters [9, 12, 20-23, 53, 55, 68-72, 88-91]; evolution of dust particles in dense clouds [111]; vibrational excitation of H₂ desorbed from a carbon surface [96]; molecular desorption from dust in star-forming regions [116]; H₂ formation on carbonaceous

grains [24]; H₂ formation on carbonaceous grains and release of mantle materials [117]; evolution of HAC grains in interstellar medium [26, 27, 107].

Laboratory Studies and Astrophysical Modelling of Other Materials

Condensation of oxides in M-star envelopes [7]; structural evolution in thermally processed silicates [110]; growth of SiC grains [49]; hydrogen cyanide polymers in the laboratory and in space [61, 63]; iron-aromatic molecule chemistry in interstellar clouds [10, 62]; gas-grain chemistry in protosolar nebula [77].

Astrophysical Ices: Laboratory Studies and Astrophysical Observations

Ion irradiation of model ices [46, 51, 76, 106]; photochemical studies [44, 94, 98]; astrophysical observations [6, 86, 99]; evidence for chemical processing in pre-cometary icy grains in circumstellar environments of pre-main sequence stars [108]; UV desorption from water ice [113]; icy grain mantles and dust/gas chemical modelling [102]; photodesorption of CO ices [38]; mantle desorption processes driven by cosmic rays [115]; water ice formation on interstellar carbon dust [25]; high density water ice and its role in formation of icy mantles [47, 48].

Interplanetary Dust Particles, Micrometeorites and Meteorites

Interplanetary dust particles: observation and harvesting in the Antarctic [65], reactions in the Earth's atmosphere [66, 67]; origin of micrometeorites and meteorites [11]; interstellar grains in meteorites [79]; laboratory comparisons of organic materials to interstellar dust and meteorites [57, 83, 84, 95]; laboratory simulation of microdiamonds in space [22]; interstellar and circumstellar grains in meteorites [3, 4, 43]; formation of iron meteorites [30]; formation of oxides in carbonaceous chondrites [35].

Other Relevant Topics

Comets as reflection of interstellar medium chemistry [33]; Pre-biotic chemistry in space [60]; Large organic molecules in the interstellar gas [56, 109]; Photochemistry in dark clouds [14-16]; Diffuse interstellar bands: Review [41]; Constraints on the identification of the diffuse interstellar bands [40]; Laboratory evidence for highly unsaturated hydrocarbons as carriers of some of the diffuse interstellar bands [31].

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