COMMISSION 14 : ATOMIC AND MOLECULAR DATA (DONNEES ATOMIQUES ET MOLECULAIRES)

Introduction

Since its creation, the Commission has been keen on activating the cross-discipline interaction between astrophysics and atomic and molecular physics. The need for a variety of atomic and molecular data has become more and more important for the recent past years. This need will certainly increase still more in the next years, due to the creation of new ground based instruments and to the launch of new space missions : they will produce large amounts of high resolution spectra from the X-rays to the infrared and millimeter wavelengths involving many atoms, ions and molecules. At the 1988 Baltimore meeting there was a general consensus that the aim of the Commission is to watch over the atomic and molecular spectral and structure data, together with the energy exchange processes in atomic and molecular physics relevant for astrophysics. In particular, the Commission is concerned by the interactions between photons and atoms (or ions or molecules), including wavelengths and line transition probabilities data, and by the interactions between particles, including atomic, molecular, ionic and electronic collision cross-sections, and by related phenomena, such as line broadening, collisional redistribution of radiation and line polarization. All these informations are essential for the interpretation of astronomical observations, such as spectroscopic diagnosis and theoretical modelling of astrophysical media.

The following working groups, which have evolved from those of past years, together with their chairmen were approved for 1988-1991 :

1 : Atomic spectra and Wavelengths standards : W.C. Martin
2 : Atomic transitions probabilities : W.L. Wiese
3 : Collision processes : J.W. Gallagher
4 : Line broadening : N. Feautrier
5 : Molecular structure and Transition data : W.H. Parkinson

WORKING GROUP 1 : ATOMIC SPECTRA AND WAVELENGTH STANDARDS

A. Laboratory Research on Energy Levels and Line Classification

Some references for data on energy levels, wavelengths, and line classifications for elements $Z \leq 28$ are sorted according to spectrum in Table 1. The references are indicated by the first letter of the first author's last name and a serial number; these short notations precede the appropriate citations in the (alphabetically ordered) reference list at the end of the report. The large extension of the observations and analysis of Fe I in the ultraviolet region by Brown et al. (1988) should be noted, and also the substantial extension of the infrared data for this spectrum by Johansson and Learner (1990). A monograph by Iglesias et al. (1988) includes all known data from the analysis of V II, with some 2800 classified lines. Ekberg et al. (1990) have classified more than 500 lines of Ca IV in the range 295-2830 Å.

Table 1 does not include references to the data compilations cited in section C of this report, and also does not include a number of papers giving data for spectra of isoelectronic sequences. The following references are organized by

D. McNally (ed.), Reports on Astronomy, Vol. XXIA, 105–136.

isoelectronic sequence :

Sequence	Spectra	Reference
He I	He I - Fm XCIX	Drake (1988)
	S XV - Y XXXVIII	Aglitsky et al. (1988)
Na I	S VI - Cu XIX	Jupén et al. (1988)
Mg I	K VIII - Kr XXV	Churilov et al. (1989)
	Ca IX - Ge XXI	Litzén & Redfors (1987)
	Ca IX - Zn XIX	Redfors (1988)
	Fe XV - Nd XLIX	Seely et al. (1988)
Al I	Ca VIII - Ni XVI	Redfors & Litzén (1989).

Martinson's 1989 review of the spectroscopy of highly ionized atoms includes experimental and theoretical results.

It must be admitted that the references in Table 1 do not go very far towards providing the new data most needed for astronomical spectroscopy. Johansson and Cowley (1988) have reviewed in detail the completeness of the available laboratory data for the spectra of the neutral, singly and doubly ionized iron-group elements scandium through nickel. Another recent survey useful as a guide to needed laboratory research covers the third and fourth spectra of vanadium through nickel (Cowley and Frey, 1988). Several papers given at a 1989 conference also review laboratory data in comparison with astrophysical needs (Hansen, 1990). With regard to ongoing research of special interest, new or extended analyses are underway for S III, IV, S VII, Ar IX, Ti XII, Cr II, Fe I, II, Co I, II and Ni I (Johansson, 1990).

Spectra of elements having Z > 28 have been omitted from Table I due to limited space. An extensive new analysis of Y II can be noted here (Nilsson and Johansson, 1990). The Atomic Energy Levels Data Center will answer inquiries from astronomers about data for spectra of all elements (see AEL).

B. Wavelength Standards and Wavelength Measurement of Special Interest

Extreme-Ultraviolet and Ultraviolet Regions. The spectrum of a platinum hollowcathode lamp is now used for wavelength calibration in both laboratory and astronomical spectroscopy. Reader et al. (1990) have published wavelengths for about 3000 lines from this source, with uncertainties of 0.002 Å or less over the range 1100-4000 Å . The wavelengths of about 150 lines of O II in the range 1074-2133 Å can be obtained with estimated uncertainties smaller than 0.005 Å by using calculated wavenumbers given by Pettersson and Wenaker (1990) on the basis of their new measurements. The absorption-spectrum observations of about 3000 Fe I lines in the 1550-3215 Å region by Brown et al. (1988) gave wavelengths with estimated uncertainties of 0.001 Å for the best measured lines. The astronomically important resonance-doublet lines of lithium-like C IV and O VI have been redetermined : Rottman at al. (1990) measured the C IV doublet near 1550 Å to about ±0.008 Å , and Kaufman and Martin (1989) give wavelengths for the O-IV doublet, λλ1032, 1038, with estimated uncertainties of 0.003 Å .

Near-Ultraviolet and Visible Region. Learner and Thorne (1988) have determined the wavelengths of some 300 Fe I lines in the range 3830-5760 Å within an estimated uncertainty of 0.001 cm^{-1} (±0.00015 to ±0.0003 Å).

Infrared Region. Johansson and Learner's (1990) table of their new measurements of Fe I in the range 7320-4712 cm^{-1} has about 360 lines. The estimated uncertainty is less than 0.003 cm^{-1} for symmetric lines.

C. Compilations of Laboratory Data and Bibliographies

Energy Levels. New compilations of energy levels have appeared for He I (Martin, 1987), for the sulfur spectra S I through S XVI (Martin et al., 1990), and for the copper spectra Cu I through Cu XXIX (Sugar and Musgrove, 1990a). Sugar and Musgrove have also compiled the energy levels data for molybdenum, Mo I through Mo XLII (1988), and their similar compilation for krypton is under review (1990b).

Wavelengths and Energy-Level Classifications. Morton et al. (1988) have critically compiled wavelengths and oscillator strengths for 179 atomic resonance lines longward of 912 Å that are "suitable for use in search lists for QSO absorption systems". Wavelengths and their level classifications have been critically compiled for all observed lines of Mg I through Mg XII (Kaufman and Martin, 1990) and Sc I through Sc XXI (Kaufman and Suger, 1988). Wavelengths with classifications, and also Grotrian diagrams, are given for high-ionization spectra of iron (Fe VIII - Fe XXVI) and copper (Cu X - Cu XXIX) in the compilations by Shirai et al. (1990a, 1990b). Observed wavelengths for the potassium-like spectra V V through Cu XI are included in the tables of Fawcett (1989). Nussbaumer et al. (1989) have compiled two short tables of wavelengths for lines that might be observed in spectra of appropriate astronomical sources as a result of Raman scattering by ground-state hydrogen and ionized helium.

Computer-Readable Experimental Data. Extensive lists of wavelengths derived from experimental energy levels are a part of the output of Kurucz's program of calculations for spectra of the iron-group elements calcium through nickel (Kurucz, 1990). Data for the first nine spectra of each element are now included. Kurucz plans to distribute these data in computer-readable form. A new multiplet table for Mn I prepared by Adelman et al. (1989) is available on magnetic tape. Most of the energy levels and wavelengths data included in publications of the NIST Atomic Energy Levels Data Center can also be supplied in computer-readable form (AEL).

Bibliographies. A bulletin on atomic and molecular data for fusion that now appears twice yearly has a bibliographic section covering papers on energy levels and wavelengths for selected elements (Smith, 1988-90). Heilig (1987) has published a bibliography on isotope shifts covering the period November 1981 to September 1986. The AEL Data Center maintains a bibliographic database (AEL).

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TABLE 1

Selected references on energy levels, wavelengths, and line classifications for spectra of elements $Z \leq 28$

He I	B1	Al X	A1	Ti VI	E1
		Al XII	G4	Ti IX	T4
B II	M1			Ti X	P2,T4
B III	B2	Si IV	B7	Ti XI	L4,T4
		Si VIII	D3	Ti XII	J5
C I,IV	J1			Ti XIII	T5
		S VI	J5	Ti XIX,XXI	M4
N V	B3,G3	S X	D3		
				V II	I1,I2
O I	C3	Cl I	C2		
O II	P1	Cl VII	J5	Mn I	T1
O VI	B3,K2	Cl VIII	J4		
				Fe I	B8,J3,L1
F VI	B4	Ar IV	L3	Fe II	J2
F VII	B3	Ar VI	L3,P3	Fe XIII,XIV	T3
		Ar VII	L3	Fe XIII-XV	T4
Ne I	I3	Ar VIII	B5,J5		
Ne IX	D2	Ar X,XIV	P4	Co XX	D1
		Ar XII	D3		
Na I	G1	Ar XVI,XVII	K1	Ni VII	V2
				Ni VIII	L5
Mg I	L2	K VIII	L4	Ni IX	V1
Mg II	F1,G2	K XI,XII,XV	P4	Ni XV	T2
Mg X	B3			Ni XV-XVII	T4
Mg XI,XII	M3	Ca IV	E2	Ni XXVI,XXVII	B6,H1,Z1
		Ca IX	L4		
Al I	B9,C2	Ca XI	R1		
Al III	B7,F1,M2	Ca XII,XIII	P4		

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W.C. Martin
Chairman of the Working Group

WORKING GROUP 2 : ATOMIC TRANSITION PROBABILITIES

The data Center on Atomic Transition Probabilities at the National Institute of Standards and Technology (formerly the National Bureau of Standards), Gaithersburg, MD 20899, USA, continues its critical compilation work and maintins an up-to-date bibliographical database. Two new data volumes containing transition probabilities for 8800 lines of the elements Sc through Mn (Z = 21-25) and 9500 lines of the elements Fe through Ni (Z = 26-28) have been published as supplements to the Journal of Physical and Chemical Reference Data (Refs. A and B). An important new source of transition probability data for the light elements--helium through neon (Z = 2-10)-- are the extensive atomic structure calculations undertaken as part of the "Opacity Project". All stages of ionization of these elements are covered, and results are now being published in J. Phys. B (see Refs. 41,94, 96, 132, 152) and in book form.

In Table 1 the important recent literature references containing atomic transition probability data which have been published since the last Working Group report of August 1987 are presented; this material is ordered according to element and stage of ionization. For brevity, the references are identified there only by the running number of the general reference list given at the end of this report. In order to keep the size of this list within the allowed space, both the spectra listed here and the references within each spectrum had to be on a selective basis. However, the NIST Data Center will supply all inclusive lists of references on specific spectra request. In the general reference list supplied with this report, the literature is ordered alphabetically according to first author. Following each reference are one or more code letters indicating the method applied by the authors. These code letters are defined as follows :

THEORETICAL METHODS :

Q - quantum mechanical (including self-consistent field) calculations.
CA - Coulomb approximation
I - interpolation within isoelectronic sequences, spectral series, or homologous atoms; also, data that are presented in graphical, rather than tabular form.

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).
H - anomalous dispersion (hook) measurements.
M - miscellaneous experimental methods (for example, Stark effect, astrophysical measurements, etc ...).

OTHER :

CM - additions or suggested revisions to data in previous articles, comments on particular theoretical or experimental methods, etc ...
CP - data compilation.
R - relative (non-absolute) oscillator strengths have been determined.
F - data on forbidden (i.e. other than electric dipole) transitions have been determined.

References for Introductory Discussion

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TABLE 1

Recent literature sources for atomic transition probability data of astrophysical interest

This table covers the 3 year period since the publication of our last IAU report (Reports on Astronomy, Volume XXA, 117 (1988); preparation date : August, 1987) to the present (July 1990). The table is arranged in alphabetical order of element symbols, with further subdivisions according to stage of ionization (I, II, etc ...). The numbers are the running numbers of the reference list following this table.

Al I : 60,144
Al II : 27,66,67,118
Al III : 106

C I : 33,37,54,61,94,148
C II : 133,152
C III : 91,136
C IV : 32,86,153

Ca I : 11,33,73,74,87,98,126,139
Ca II : 33,57,58,107,112,145

Cr I : 33,68,99
Cr II : 92,93,99,105

Fe I : 19,24,33,40,46,52,104
Fe II : 13,20,36,38,46,63,105,116,135
Fe III : 39,46
Fe X : 46,62

He sequence : 30,41,78,79,122

He I : 48,80,89,121,132

Hg I : 2,7,31,66,97,102,103,110,123,138
Hg II : 8,16,17,75,123

Mg I : 4,25,26,33,73,76,108,109,137
Mg II : 3,49,113,128

N I : 33,53,70,155
N II : 6,22,37,69,94,100,129,149
N V : 129

Na I : 14,23,29,33,44,60,71,81,82,88,111,114,128,154

Ne I : 47,60,125,141,146
Ne II : 18,77

Ni I : 15,33,46,117
Ni II : 46,105,117

O I : 33,34,35,64,65,70,85,90,142,150
O II : 5,28,42,69,115,129,130
O III : 37,69,83,84,96,100,115,127,129
O IV : 115,129

S I : 33,43
S II : 45,119,129,143

Si I : 9,33,124,131,140
Si II : 95
Si III : 27,66,120

Sr I : 10,21,50,73,74,101,147
Sr II : 21,51

Ti I : 33,59,99
Ti II : 56,58,99,105

V I : 99
V II : 12,99,105,134

Y I : 55,124
Y II : 55,101,124,151

Zn I : 1,66,72,131

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WORKING GROUP 3 : ATOMIC COLLISIONS

In the spirit of preceding reports of this Working Group, an effort will be made to restrict references to articles containing data in the form of cross-sections, collision strengths, and/or rates. All references are given in a general list at the end of this report. In the tables, each reference is annotated with a (T) theoretical, (E) experimental, or (A) analysis. An expanded version of this report giving tables for each of seven subtopics (electron-impact excitation of atoms and atomic ions; electron-impact ionization of atoms and atomic ions; electron-ion recombination; electron-collisions with molecules including excitation, ionization, and dissociation; non-reactive energy transfer in heavy particle collisions; heavy particle collisional charge transfer and ionization; and reactive collisions) is available from the author.

Two noteworthy books honoring Alex Dalgarno appeared in 1988 (1) and 1990 (2). Although the chapters therein are not data reviews in the strict sense, they do summarize recent developments in the fields of electron and heavy-particle collisions, ion-molecule and neutral-neutral reactions and charge transfer and contain useful reference lists.

1. Electron impact excitation of atoms and atomic ions

New developments in theoretical techniques complemented by continuing advances in computer technology have resulted in a wealth of new data in this area. A recent review summarizes and evaluates calculations of collision strengths

and cross-sections for atomic ions (3). Also, the next step planned by participants in the Opacity Project (4) is massive calculations of collision strengths for astrophysically abundant ions. A new way of critically assessing and compacting data for electron impact excitation of positive ions has been developed (5), and data for Ar XVI, Mg X, and Sr II have been analysed (5 - 7). Another report compiles and evaluates measurements of electron impact excitation of atoms and atomic ions (8). Fabrikant et al. (9) reviewed data for electron impact formation of metastable atoms. Articles reporting individual studies for neutral atoms are listed in Table 1. Theoretical data for ions can be identified from the Pradhan review (3) or from the expanded version of this report.

TABLE 1
References on electron impact excitation of neutral atoms

Ba I	10(T)
H I	11(T), 12(T), 13(T), 14(T), 15(T), 16(T)
He I	17(A), 18(E), 19(T), 20(T)
Li I	21(T)
O I	22(T), 23(T), 24(E)
S I	25(T)

2. Electron impact ionization of atoms and atomic ions

Lennon and coworkers (26) have recently published a collection of recommended data on electron impact ionization for atoms and ions with Z between 9 and 28 inclusive. Articles giving new data on electron impact ionization ions with Z up to 28 are in Table 2.

TABLE 2
New references giving data on electron impact ionization cross-sections supplementing the work of Lennon et al. (26).

Al I	27(E)	Ne I	29(E)
Al II	28(E)	Ne II	31(E)
Ar I	29(E), 30(T)	Ni II	43(T)
Ar II	31(E)	Ni IV	43(T)
Ca I	32(E)	Ni VI	43(T), 44(E)
Fe I	27(E)	Ni VII	43(T), 44(E)
Fe XVI	33(T), 34(T)	Ni VIII	43(T), 44(E)
Fe XXVI	35(T)	Ni IX	43(T), 44(E)
H I	36(E)	Ni XIII	43(T), 44(E)
H-like ions	35(T), 37(T)	Ni XV,XVII	43(T), 44(E)
He I	29(E), 38(T), 39(E), 40(T)	Ni XVIII	45(T)
		Ni XXVIII	35(T)
Li III	41(E)	O VI	46(E)
Li-like ions	42(T)	S I	27(E)
Mg I	27(E)		

3. Electron-ion recombination

The last three years have seen major advances in both measurements and calculations of data on dielectronic recombination. These were reviewed by Hahn

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and LaGattuta (47). Romanik (48) computed dielectronic recombination rates for C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, and Ni ions in the He, Li, Be and Ne isoelectronic sequences. Individual studies are listed in the expanded version of this report.

New results have been reported for radiative recombination for the Rb, Cu and Ag isoelectronic sequences (49), N V and O VI (50), Ni XXVII and Ba LV (51) and for hydrogenic ions (52,53).

Mitchell summarized the dissociative recombination of molecular ions (54) and Yousif and Mitchell (55) reported recombination cross-sections in HeH^+.

4. Electron collisions with molecules including excitation, ionization and dissociation

A recent review covers cross-sections for electron collisions with hydrogen molecules and molecular ions (56). Some other articles dealing with electron-molecule collisions are for H_2 (57(T), 58(E), 59(E)), for CO (60(E), 61(E)), H_2O (61(E), 62(T)), NH_3 (62(T), 63(E), 64(E)), OCS (64(E)), H_2CO (65(T)), CH_4 (61(E) 66(T), 67(E)).

5. Non reactive energy transfer in heavy particle collisions

In an important new reference Phelps summarizes cross-sections for excitation and ionization collisions of H^+, H_2^+, H_3^+, H, H_2, and H^- in H_2 for energies from 0.1 eV to 10 keV (68). Doyle gives proton collisional excitation cross-sections for Be-like ions (Z = 6, 7, 8, 9, 10, 12, 14, 16, 18, 20, 26) (69). Flower has reviewed molecular collision processes in interstellar clouds (70). He has also reviewed atomic and molecular processes in interstellar shocks (71). Bogdanov and co-workers review the theory of vibrational-rotational excitation of poly-atomic molecules (72). Reports of other studies are listed in the expanded version of this article.

6. Heavy-particle collisional charge transfer

Recent charge-transfer reviews cover hydrogen atoms and ions colliding with gaseous atoms and molecules (73); H, He, and H_2 in collisions with C^- and O^- ions (74) and electron capture by neutral and charged particles in collisions with He (75,76). Other recent charge transfer studies are listed in Table 3.

TABLE 3
References giving data on charge-transfer reactions

H(+)	H	77(E)	H	Be(3+)	99(T)
H(+)	H(2s)	78(T)	H	C(3+)	100(T)
H(+)	H(-)	78(T), 80(T)	H	C(4+)	99(T), 101(E)
H(+)	H2	81(E/T)	H	C(6+)	98(T), 99(T)
H(+)	H2	77(E), 82(T)	H	C(6+)	102(T)
H(+)	H2	83(T), 84(E)	H	N(3+ -5+)	103(E)
H(+)	He	85(E), 86(E)	H	N(5+)	98(T)
H(+)	He(+)	87(T)	H	Ne(8+)	98(T)
H(+)	C(+), N(+)	88(E)	H	O(2+)	104(T)
H(+)	Na	89(E), 90(T)	H	O(4+)	105(T)
H(+)	H2O	91(E)	H	O(6+)	98(T)

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H(+)	CH4	92(E)	H	O(8+)	98(T)
H	H(+)	77(E)	H	Si(4+)	105(T)
H(2s)	H(+)	78(T)	H2	Ar(+)	106(E)
H	H	77(E), 93(T)	H2	Ar(8+)	107(E)
H	H(-)	77(E), 94(E)	H2	He(+)	107(E)
H	H2	77(E)	H2	He(2+)	83(T)
H	He	86(E)	H2	C(+)	108(E)
H	He(+)	95(T)	H2	C(4+)	101(E)
H	He(2+)	87(T)	H2	N(2+, 3+)	109(E)
H(2s)	He(2+)	78(T)	H2(+)	Na	89(E)
H(2s)	Li(3+)	78(T)	H2,D2	O(2+)	110(E)
H	Aℓ(+)	96(T)			
H	Aℓ(3+)	97(T)			
H	Ar(8+)	98(T)			

7. Heavy-particle reactive collisions

A major source of rates for neutral reactions is the National Institute of Standards and Technology (NIST) Chemical Kinetics Database (111) which includes 12 000 records containing data on 5 000 reactions for 2 400 compounds.

A general collection of ion-molecule reaction rates (112) lists 9 300 rate constants for bimolecular and termolecular reactions of both positive and negative ions with neutral molecules.

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Jean W. Gallagher
Chairman of the Working Group

WORKING GROUP 4 : LINE BROADENING

The interest in the field of line broadening has continued to grow over the last three years, mostly stimulated by the more recent astronomical observations or by the preparation of space investigations. It is not the purpose of this report to be exhaustive, so we will simply give results relevant for astrophysical purposes and indicate some new directions for future research in this theme.

1. Line broadening in low to moderately dense plasmas

1.1. STARK BROADENING OF NON HYDROGENIC LINES

As indicated in the last report, the Opacity Project constitutes a major effort to produce extensive calculations of atomic data required for opacity determination. This work includes Stark broadening of atoms and ions. For non hydrogenic atoms or ions, the profile is Lorentzian with a width and a shift given in terms of scattering matrix elements. Use of the very accurate R-matrix method is well adapted to the determination of the widths and the shifts of the lines involving low excited states. But this approach cannot be extended to transitions between highly excited states and approximate formulae have been obtained. Important results for the line profile parameters have been published on CIII (1), Li-like and Be-Like ions (2), neutral atoms of He, C, N, O (3).

A complementary and interesting direction for research concerns the regularities of the Stark broadening parameters within spectral series or homologous atoms or ions (4-9). The following table presents results for many transitions of astrophysical interest. The table is arranged in alphabetical order of element symbols with subdivisions according to stage of ionization. The numbers refer to the running numbers of the reference list.

TABLE

Ar I	: 10,11,12,13	N II	: 33
Ar II	: 14,15	N III	: 33
Ar III	: 16	N IV	: 33
Ar IV	: 16	N V	: 33,34
C II	: 17	Ne I	: 35
C III	: 17	Ne II	: 36
C IV	: 17,18,19		

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Cℓ I	: 20	O I	: 37,38
Cℓ II	: 20	O II	: 39
		O III	: 39
Cu I	: 21	O IV	: 39
Cu II	: 21	O V	: 39
		O VI	: 40
Fe I	: 20,22		
Fe II	: 23	S I	: 41
Fe III	: 24	S II	: 41
Ge I	: 25	Si II	: 42
He I	: 26,27,28,29	Xe I	: 31,32
		Xe II	: 31,43
K I	: 30		
Kr I	: 31,32		
Kr II	: 31		

The effetc of the Debye shielding has been revisited (44).

1.2. HYDROGEN AND HYDROGENIC LINES

It is now well established that the ionic broadening of hydrogen and hydrogenic lines cannot be described in all circumstances in a quasistatic approach. In fact, ion dynamics play an important role in the central part of the lines and the quasistatic ion assumption is only valid for the wings at low or moderate densities or for the major part of the profile at relatively high densities. The notion of low or high densities depends on the temperature of the plasma, the emitter (neutral or ionic), the line studied (45). Fortunately, at low densities the Doppler broadening is mostly dominant in the center of hydrogen or weakly ionized ionic lines so that the usual static approach for ionic perturbers gives satisfying results, the electronic broadening being treated by unified theories. In this context, new important results for the He II lines have been published (46,47). Extensive calculations are in progress in the framework of the Opacity Project.

New accurate results have been also obtained from laboratory measurements for Hβ (48-50).

In spite of these results, much work remains to be done in the future particularly for Lyman, Balmer and Paschen series.

2. Hot and dense plasmas

The study of spectral line profiles in hot and dense plasmas remains a subject of major interest for astrophysical purposes, specially for the physics of white dwarfs, neutron stars and the internal structure of stars. Research in this field is greatly stimulated by inertial confinement studies. Some of the more important problems can be found in the Proceedings of the Workshop "Spectral line formation in plasmas under extreme or unusual conditions" (51).

For hot and dense plasmas, simultaneous strong interactions between the radiator and the surrounding ions may occur. The relatively high velocities of the perturber prevent to consider these interactions as static and many efforts have been devoted these last years to this many body dynamical problem. Most of the work interesting for astrophysics concerns the hydrogen atom and hydrogenic

ions.

Ion dynamic effects are well taken into account by numerical simulation methods (52). However such calculations are computer time consuming and may be considered as references for approximate methods. So, it is important to develop other theoretical approaches and there is a real interest in this field. Many theories are actually developed such as a generalization of the unified theory (53) or the development of the Model Microfield Method. This last method seems to be particularly adapted to this problem and many important results are expected for the next years. Fine structure splitting should be taken into account.

The shift of hydrogenic ion lines in plasmas, important in dense plasmas (54), becomes negligible in most of the stellar atmospheres conditions.

Another problem concerns the strong correlation effects which appear between the internal structure of the radiating ion and the perturbers. The physical limit between bound and free states becomes a function of the density and the temperature (55). This leads to the disappearance of upper members of spectral series in dense plasmas (56). Such studies improve the Inglis Teller formula.

Interesting effects arising from external electric fields have been also investigated (57).

Experiments on the Hα line of hydrogen (58), on the Balmer α, β (59) and Paschen α (60) lines of He II and on the Hα, Hβ and Lδ lines of C VI (61) have been carried out.

3. Line broadening by foreign gases and molecular line broadening

Not much work has been done in atomic line broadening. In fact, the theory is well known, and methods describing the dynamics of the collisions are efficient but quantitative results mainly depend on the accuracy of the relevant interatomic potential energies. A constant effort concerning interatomic potentials remains, but there is actually no general agreement between the theoretical and the experimental results. Besides methods giving the general trends in neutral atom broadening (62, for alcali), there is a need for accurate results for specific applications (broadening by hydrogen atoms for example).

At high perturber densities, simultaneous strong interactions contribute to the profile. Temporary molecules are formed during the collision. The existence of such transient molecules (H_3, H_3^+) have been proved in the IUE spectra of white dwarfs (63).

Concerning molecular broadening, many theoretical or experimental results hve been obtained, greatly stimulated by new spatial observations of planetary atmospheres. We will quote particularly broadening of water vapor (64), CO by H_2 and N_2 (65,66), ethane by H_2 (67), CH_3D by H_2 and N_2 (68), germane by H_2 (69), acetylene by H_2 and N_2 (70) and self broadening of CO_2 (71).

It has been shown that line coupling induced by collisions leads to important modifications of the absorption in the microwindows of the self and N_2 broadened ν_3-CO_2 fundamental vibration rotation band (72).

The density dependence of the 5 μm infrared spectrum of NH_3 has been investigated (73), discrepancies remain probably due to NH^+_3 dimers. Many important results have been obtained on the broadening and the shifts of the ν_4 fundamental band of CH_4 (73-77) and on the ν_2 vibration band of NH_3 (78). In spite of this

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effort, many work remains to be done for the preparation of future observations and a particular attention has to be paid to systematic studies on the temperature dependence of the broadening.

Many rototranslational collision induced spectra have been determined both experimentally and theoretically (79-91). The existing model line shapes have been reconsidered (83,84) and the use of very accurate ab initio binary induced dipole surfaces has led to profiles in close agreement with existing measurements of binary spectra (90). Accurate synthetic spectra of Jupiter in the region of 5 μm have been obtained (92).

In cool and dense environments, some spectra exhibit 3-body contributions. The problem of three body components have been recently investigated (93,94). New experimental studies on the density dependence at low temperature are needed for probing such many-body interactions.

The far infrared rotational absorption spectrum of HD has recently been the subject of several studies and collisional interference between allowed and collision-induced transition has been pointed out (95-97).

4. Line broadening and related topics

The problem of interference in the spectra of overlapping lines has been revisited (101,102).

There has been some new work concerning the computation of the Voigt function (103-105).

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Nicole Feautrier
Chairman of the Working Group

WORKING GROUP 5 : MOLECULAR STRUCTURE AND TRANSITION DATA

Basic reasearch in molecular spectroscopy has continued to increase over the past three years. The spectral range extends from millimeter to extreme ultraviolet wavelengths. This report has been compiled from edited contributions sent to me in the summer of 1990.

During the past three years, nineteen new molecular species have been identified in interstellar clouds and circumstellar shells, often with the astronomical detection preceding or in conjunction with the laboratory study. Frank J. Lovas (NIST, Gaithersburg) cites the increase in the number of hydrocarbon radicals observed in the microwave region. The number has been augmented with

the detection of CH_2 (1). The spectrum of the ring form of C_3H has been observed both in laboratory and astronomical objects (2), (the linear C_3H radical had been identified previously). New laboratory studies of the carbene ring C_3H_2 have appeared by Vrtilek, (3) and Bogey (4), who also report spectra for the ^{13}C and deuterated isotopic forms which have now been detected in Taurus molecular cloud-1 (5). Similarly, vibrationally excited C_4H has been identified by means of new laboratory measurements by Yamamoto (6). Turner (7) has identified C_4D towards the TMC-1 cloud based on laboratory measurements od Woodward (8). Spectra of the largest hydrocarbon radicals C_5H and C_6H have been observed only in astronomical sources. Further laboratory work is needed. The electric dipole moments for many of these radicals are also lacking. Citations and transition frequencies for these species and the other hydrocarbons studied in the laboratory may be found in the recent review by Lovas and Suenram (9).

Laboratory and astronomical studies of new silicon-carbon species have also appeared recently. The microwave spectrum of SiC has been detected by Gottlieb (10) and identified in IRC+10216. Subsequently the $Si^{13}C$ species and vibrationally excited state spectra were analyzed by the same group (11). While SiC_2 was originally identified in 1984, its laboratory microwave spectrum has only been obtained recently by Gottlieb (12) and similarly for measurement of its dipole moment (13). A combined report of the laboratory and astronomical spectrum of SiC_4 has appeared from Ohishi (14). In 1986, a report by Saito (15) attributed several interstellar features to HSiCC or NCSi, but this has not yet been confirmed by laboratory studies.

Two new carbon-sulfur species have been characterized in laboratory studies, i.e., C_2S and C_3S (16), and in the reports it has been shown that a number of previously unidentified astronomical features could be explained as arising from these molecules.

Searches for inorganic diatomic species have resulted in the identification of AlF, AlCl, NaCl and KCl (17) and PN has been identified by Turner and Bally (18) based on much earlier laboratory studies. Another unusual species recently identified in the TMC-1 and SgrB2 is the cyanomethyl radical (CH_2CN) (19) based on laboratory measurement of Saito (20).

While many of the radio-astronomical lines have been clearly identified, there remain about 700 unidentified features which await association with a molecular precursor. These observations and the firmly established molecular transitions are summarized in the most recent revision of the tabulation of recommended rest frequencies for interstellar molecules by Lovas. P. Qin-Zeng (Purple Mountain Observatory, P.R. China) has reported calculations of the total energies, transition frequencies, and A-values of the A-type CH_3OH molecule (21).

Takeshi Oka (Departments of Chemistry, and Astronomy and Astrophysics, University of Chicago) has reported the observation in the laboratory of the infrared spectrum of the hot bands (22), the first overtone band (23), and the second overtone band (24) of H_3^+. They provide crucial information for the identification of the 2μm emission spectrum of H_3^+ recently observed in Jupiter (25,26) and other laboratory spectrum (27).

Oka and Geballe (28) have observed the 4μm emission band of H_3^+ which indicated the LTE behavior of this species in the Jovian ionosphere and temporal variation of the effective temperature.

Oka and colleagues have observed and characterized in the laboratory, spectra of other molecular ions such as $C_2H_3^+$ (29), HeH^+ (30), NH_2^+ (32); $HCCH^+$ and its isotopic species which are all of great astrophysical interest.

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A.R.W. McKellar has reported results of spectroscopy in the ultraviolet, visible infrared, and microwave regions from the Herzberg Institute of Astrophysics.

Extensive work has continued on the spectra of polyatomic molecular ions in the infrared region, including NH_3 (33,34), HCO^+/HOC^+ (35,36), $H_2C\ell^+$ (37), H_3 and its isotopes (38,27,39), CH_3CNH^+ (40), C_2H_3 (41,42), SH_3 (43), H_2COH (44), $HOSi^+$ (45,46), and HN_2^+ (47). A highlight in their work on ions was the observation noted above of the spectrum of H_3^+ in emission from auroral hot spots on Jupiter (25). Other unstable polyatomics that were studied include NH_2 (48, 49, 50, 51), C_2H (52,53), HNO (54), HCO (55), NCO (56), C_5 (57,58), CH_2 (59,60), and LiOH (61). A new program of accurate high-resolution infrared intensity measurements and analysis was initiated with studies of CO_2 bands of atmospheric interest (62,63,64,65). Other stable polyatomics studied in the infrared include glyoxal (66), D_2S (67), SCCCS (68), H_2O_2 (69,70), C_2H_2 (71), H_2CO (72), CH_3OH (73,74), C_6H_6 (73,74), C_6H_6 (75), CH_3SH (76), and CH_4 (77).

In the infrared region, collision-induced and dimer vibration-rotation spectra involving the molecules H_2 (78,79,80,81), and N_2 (82,80) were obtained. Experimental work on HCℓ dimers (83,84) and theoretical work on HF dimers (85,86) was also carried out.

A recent theoretical study of quintet states in N_2, (87) provided convincing evidence for the assignment of the Herman infrared bands to the transition $C\ ^5\Pi_u$ - $A'\ ^5\Sigma_g^+$. Huber and Vervloet (88) have done a rotational analysis of the Herman infrared bands which confirms the theoretical analysis.

Electronic spectra have been studied for CO (89), NO (90,91), NH^+ (92), SiF (93,94) and N_2 (95).

In the Harvard-Smithonian Center for Astrophysics (Cambridge, Ma), M. Kirby and colleagues have carried out ab initio calculations of the low-lying $^3\Sigma^-$, $^3\Pi$ and $^5\Sigma^-$ states of NH (96,97). Photodissociation cross-sections and interstellar photodissociation rates have been reported. Predissociation through low-lying levels of the $A^3\Pi$ state have been discussed and it is shown that the $^5\Sigma^-$ cannot cause the predissociation.

Theoretical calculations of five low-lying states of $^1\Sigma^+$ and $^1\Pi$ symmetry have been reported (98,99,100). Electronic potential energy curves, wavefunctions, and dipole transition moments were calculated using multiconfiguration self-consistent field plus configuration interaction methods (MCSCF-CI). Calculated oscillator strengths and radiative lifetimes have been given. A new Rydberg state of CO, the $W^1\Pi$ state, the first in a series converging to the $A^2\Pi$ excited state of CO^+, has been characterized and the absorption oscillator strength from the $v''=0$ level of the ground state calculated. Rosenkrantz and Kirby (101) have reported on calculations of the metastable $^1\Delta$ and $^1\Sigma^-$ states of CO which have very long-lived $v=0$ levels.

A review of photodissociation processes in diatomic molecules of astrophysical interest by Kirby and Van Dishoeck has been published in Advances in Atomic and Molecular Physics (102).

W.H. Parkinson and colleagues at the Center for Astrophysics have reported the results of high resolution studies in the VUV region on molecules of interstellar and atmospheric interest.

Because of the importance of CO as a tracer of large scale distribution of molecular gas in galaxies, there is considerable interest in and need for basic, quantitative spectroscopic data for CO at vacuum ultraviolet wavelengths. How-

ever, at present, the identification and analysis of CO spectral features at wavelengths between 91.2 and 111.8 mm are incomplete. Recent work by Eidelsberg and Rostas (103) has significantly extended the analysis and presents a set of molecular constants for the predissociating excited states. Letzelter (104) has used fluorescence yields to estimate the probabilities of photodissociation for individual vibrational levels. Stark (105) has used the spectroscopic facilities at the Photon Factory to obtain high-resolution $\lambda/\Delta\lambda \cong 1.5 \times 10^5$ photoabsorption coefficient data for CO between 91 and 100 nm.. The Photon Factory has been used to obtain photoabsorption coefficient data for C_2H_2 |140-200 nm|, HCℓ |C(0) and C(1) - X(0) bands|, and CO |E(0), E(1), C(0), and C(1)-X(0) bands|.

Yoshino and colleagues (Center for Astrophysics) have completed wavelength and band oscillator strength measurements of the Schumann-Runge bands of $^{18}O_2$ and $^{16}O^{18}O$ (106,107, 108,109).

R.S. Friedman (110) has calculated the oscillator strengths of the Schumann-Runge bands of $^{16}O_2$, $^{18}O_2$ and $^{16}O^{18}O$, discussed the dependence of band oscillator strength on reduced mass, on vibrational level, and the variation of rotational oscillator strength with rotational quantum number. The calculations agree with the measurements by Yoshino.

The predissociation line widths of the Schumann-Runge bands of $^{16}O_2$ (111), $^{18}O_2$ and $^{16}O^{18}O$ (112,113) have been derived from their absolute cross-sections. Band oscillator strength measurements of the hot bands of the Schumann-Runge system have also been completed (114). Two independent measurements of the absorption cross-sections of the Herzberg continuum of O_2 (Reims and CFA) (115) have been combined to present more accurate results. Absolute cross-sections of O_3, in the wavelength region 238-335 nm, and its temperature dependence have been measured (116,117).

J.H. Carver and B.R. Lewis (Australian National University, Canberra) have reported a number of significant spectroscopic studies of O_2, using VUV absorption and fluorescence methods (118,119), and of valence-Rydberg interactions using coupled equations (120,121). The theoretical techniques appear to explain completely the complex window region spectrum of O_2, and to provide valuable information on many hitherto unobserved repulsive states of O_2.

Emission bands of N_2 in the VUV region have been studied by Roncin, Launay and Yoshino (122,123) and most of the bands have been assigned in connection with absorption bands of N_2. P.K. Carroll reports from the University College Dublin that VUV spectrum of $^{15}N_2$ has been measured and analyzed from plates taken on the 10-m vacuum spectrograph in NRC (Ottawa). Configuration interaction effects between Rydberg and non-Rydberg states have been studied (124,125). In emission photodissociation in the B state of the $^4S + {}^4S$ limit has been investigated in high resolution and fragmentary structure in vibrational levels above the limit has been analyzed and interpreted (126). François Rostas (Observatoire de Paris-Meudon) has reported additional work on CO $A^1\Pi$ perturbations. The work provides a complete model of the $A^1\Pi$ and adjacent triplet and singlet states (127).

The model has been used to analyze lifetime measurements (128) and to interpret spectroscopic data concerning the e $^3\Sigma^-$, d $^3\Sigma^+$ states (129) and the $D^1\Delta$ state (130).

A comprehensive analysis of the spectroscopic data available in the ground state X $^1\Sigma^+$ leads to a new determination of its molecular constants and to very accurate predictions of the microwave and infrared transition frequencies (131) that could now be used as secondary standards in the microwave and submillimeter domain.

Rostas reported that an Atlas of H_2 emission lines between 78 and 168 nm has been completed. It comprises 12265 lines, 90% are assigned with relative photoelectric intensities.

A complete model of the B and C states has been established taking into account the non-adiabatic interactions (132). A catalog of all transitions in the Lyman and Werner systems has been established taking into account interactions between the B, B', C and D states. Line positions, intensities, and photodissociation probabilities up to J=30 are provided. The structured emission continuum associated with the photodissociation of vibrational levels of the B and C states measured after synchrotron radiation excitation is accurately predicted (133).

Rotationally resolved bands of CO_2 have been observed, superimposed on the photodissociated continuum between 180 and 200 nm. The spectrum is being analyzed (C. Cossart-Maggos, Orsay) in conjunction with ab initio calculations (P. Rosmus, Frankfurt and N. Feautrier, Meudon).

The direct and stepwise double ionization of PAH molecules followed by Coulomb or covalent fragmentation has been studied on naphtalene, azulene and other small model molecules (134). The attribution of diffuse interstellar bands to PAH's has been tested by calculating band contour for vibronic bands. The first results do not match observations (135).

R.W. Nicholls (Center for Research in Earth and Space Science, York University), has reported on his experimental and theoretical/modelling programs. A shock-tube excitation study in the Blue and IR systems of NbO has been undertaken by Gertner and Nicholls (136). Many new bands have been excited and revised molecular constants have been determined. A similar extensive program has been carried out on bands of SiH and SiN using OMA detection of shock-tube spectra (137). A program of interferometric spectroscopic "hook method" studies on the atmospheric absorption bands of O_2 has been started.

Considerable effort has been expended to enhance the extensive suite of spectral synthesis codes which they have developed to realistically simulate, on a line-by-line basis, emission and absorption spectra from the EUV to the microwave regions. Recent work includes significant improvement (138) of their earlier simulation of the O_2 Herzberg system (139). Realistic account has also been taken of particulate scattering contributions to the microwave extinction spectrum of the atmosphere in the 80GHz region and of the molecular and particulate contributions to atmospheric extinction in the region 0-1000GHz (140). Studies have also been made of the Franck-Condon sum rules for free-bound molecular transitions (141).

The Berkeley laboratory program (John Phillips, Astronomy Dept. and Sumner Davis, Physics Dept.) has continued to be directed towards measurement and analysis of molecules of astrophysical interest. In addition, computer codes have been developed for rapid data processing of Los Alamos and Kitt Peak Fourier transform spectrometers. They make possible to use of all of the Berkeley codes for data reduction, analysis, fitting, and plotting operations on IBM-compatible PC's.

The Phillips C_2 system has been observed in the spectral region 3300 to 6500-cm^{-1}. Three new bands, and additional lines of the (0-2) have been observed (142). Improved molecular parameters have been calculated for the Balik-Ramsay system (143).

Spectra of CaCℓ have been produced in a King furnace under conditions of LTE. Band oscillator strengths for the Δ v=0 bands of the Red and Orange systems have

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been determined. Franck-Condon factors have been calculated for these bands and the D-X system (144)

The work on the transition strength of the A-X and B-X systems in CaH has been partially completed . The analyses of the infrared system of FeH has been completed (145,146). Analyses of the spectral features in the more complex green and blue regions have been stated, with promising results. Observed isotope shifts have shown that a band at 7000 Å is not produced by FeH, but most probably FeH_2.

Three different sources have been used to produce the Meinel OH and OD bands in the infrared (147,148,149). The complex spectrum of TiCl in the 400 nm to 420 nm region has been photographed at the highest possible dispersion and measured. Four band systems have been identified and the strongest two analyzed (150).

Some differences of interpretation have occured about the placement of energy levels of ZrO. A set of levels based on the best available data has been constructed (151).

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