

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

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In recent years the interaction between astrophysics and atomic physics has entered a new stage. On one hand, increasingly powerful, high resolution astronomical spectrometers and other observational instruments, especially those for recent space and astronomy missions, have created vastly increased demands for more detailed and more accurate data on atomic and molecular processes. On the other hand, the advent of large-scale computing capabilities has been an important development for the atomic physics community, giving it opportunities to embark on comprehensive data generation projects that were unthinkable until recently. Indeed, several huge data projects have now come to successful conclusion. These projects have not only generated vast amounts of new data, but have also in many cases far surpassed the earlier data in their accuracy.

A principal task of this commission is to inform the astrophysics community of these new developments and provide assessments and recommendations. By its active participation in several recent and planned Joint Discussions with other IAU commissions, and by its sponsorship of relevant IAU workshops, this commission is providing the astrophysical community with information on the vast new atomic physics data capabilities that have been generated. Also, the commission provides the working group reports appearing below which highlight these new developments and list all important recent literature references in a convenient, annotated manner. The commission has expanded its scale of data gathering activities by adding a new working group on molecular reactions on solid surfaces and by adding in the collision part a section on rate coefficients for chemical reactions. The commission is fortunate to have engaged some energetic working group chairpersons for this task.

WORKING GROUP 1: ATOMIC SPECTRA AND WAVELENGTH STANDARDS

W. C. Martin, Chairperson

An extensive review of atomic spectroscopic data for astrophysics as available in 1991 has been published (Martin 1992). The references cited here are limited mainly to publications for the period 1991-1993 that include data for the elements having $Z \leq 30$. Table 1 shows most of these references sorted according to spectrum. The references are designated by the first letter of the first author's last name and a serial number; these designations precede the appropriate full citations in the reference list at the end of this report.

A. Energy-Level Analyses, Line Classifications.

A few of the references comprise extensive new observations and analyses of particular spectra included in Table 1. Persson *et al.* (1991) give some 750 classified lines of Ne III in the range 430–12000 Å; their energy levels can be used to obtain new Ritz-principle extreme UV wavelengths down to almost 200 Å, with uncertainties smaller than 0.001 Å. Ekberg's (1993) investigation of Fe III has almost doubled the number of classified lines to about 3200, mainly in the range from 600 to 2100 Å. The complete line list resulting from an extension of the Ni III analysis by Garcia-Riquelme and Rico (1992) covers the range 1290–8680 Å. Forsberg's (1991) revision and extension of the Ti I analysis yielded more than 3300 lines in the range from 2000 Å to 5.5 μm. Similar research on Ni I by Litzén *et al.* (1993) has given about 2000 classified lines from 1700 Å to 5.35 μm. Most of the resulting level values for both Ti I and Ni I were determined from high-accuracy Fourier-Transform spectroscopy (FTS); the typical uncertainties in the range 0.002 to 0.005 cm⁻¹ also apply to transition wavenumbers calculated from these levels.

TABLE 1

Selected references on energy levels, wavelengths, and line classifications for spectra of elements $Z \leq 30$

C I	G3	Ar I	B1	Co I	P1
		Ar VI	R1	Co VIII-XXVII	S2
N III	B4	Ar VII	B6	Co XIII	S8
N IV	B5				
		K VII	L1	Ni I	L2,P1
O I	Z2			Ni III	G1
O II	M1,M2,W1	Ca I	G3,U1	Ni X-XVIII,	S9
O IV	B4	Ca VIII	R2	XX-XXVI	
O V	B5			Ni XIV	S8
O VII	I1	Ti I	F1,P1	Ni XVI	P3
		Ti X	P3	Ni XVI,XVII,	H1
F V	B4,E1	Ti XII	W2	XXI-XXIII	
F VI	B5				
		V I	P1	Cu X-XXIX	S3
Ne III	P2	V VI-XXIII	S5	Cu XIV	K4
		V XIX-XXII	B3	Cu XV	S8
				Cu XVI	S7
Mg I-XII	K1				
Mg I	A1,G3,S1	Cr I	B2		
Mg II	B7	Cr II	C3	Zn III	G2
Mg VIII	R2	Cr V-XXIV	S6	Zn XV	K4
		Cr XVI-XXII	S10	Zn XVI	S8
				Zn XVII	S7
Al I-XIII	K2				
Al I	B8	Mn VII-XXV	S4		
Al II	C2				
		Fe I	G3,J2,N1, N2,N3,O1, P1,Z1		
Si I	G3				
Si VI	R2,T1,T2				
Si VII	R2				
		Fe II	N1,N2,R3		
S I-XVI	K3	Fe III	E2		
S III	J1	Fe XII	S8		
S VI	W3	Fe XIV	P3		
S VIII	R2	Fe XXV	D1		
Cl I	C1				
Cl VII	W3				

Recent investigations of Fe I and Fe II are based on, or include, FTS measurements of a hollow-cathode spectrum. Johansson and Learner's (1990) analysis of Fe I in the infrared yielded about 360 classified lines, and Nave and Johansson's (1993) further extension of this analysis includes some 2200 classified lines between 1700 Å and 5 µm. Improved wavenumbers for many Fe I lines can also be obtained from the new values given for 442 levels by O'Brian *et al.* (1991). Rosberg and Johansson (1992) give 220 newly classified Fe II lines in the 9350-10670 cm⁻¹ range.

A considerable amount of ongoing work on the first and/or second spectra of iron-group elements is centered at the University of Lund (Johansson 1993) and at Imperial College, London (Learner 1993); reports from these laboratories mention spectra of Ti, V, Cr, Mn, Fe, and Co. Most of the new observations include both FTS and high-dispersion vacuum-UV measurements, with several of the investigations involving collaborations with other laboratories.

A reference to Geller's (1992) list of solar lines in the 5000–600 cm⁻¹ infrared region is included in Table 1 for C I, Mg I, Si I, Ca I, and Fe I. These solar observations made during the 1985 ATMOS experiment yielded spectra that may include more extensive and/or more accurately measured wavelengths for some

atomic species than any available laboratory data. Similarly, the wavelengths of several infrared coronal lines as determined by Reconditi and Oliva (1993) from spectra of a planetary nebula are the most accurate available values.

Recent high-resolution observations of the spectra of chemically peculiar stars with the Hubble Space Telescope have stimulated laboratory research on the spectra of a number of elements having $Z > 30$. The current program at Lund, for example, includes new measurements and analysis of Zr II, Nb II, Mo II, Ru II, Pd II, Ag II, Ir II, and Au II (Johansson 1993), all of which are known or expected to be present in the spectrum of the B_p star χ Lupi (Leckrone *et al.* 1993). Recently published papers on Ru II (Joueizadeh and Johansson 1993), Pt II (Sansone *et al.* 1992, Blaise and Wyart 1992), Pt III (Ryabtsev *et al.* 1993), Au II (Wyart *et al.* 1992), and Hg III (Wyart *et al.* 1992, Sansone *et al.* and Reader 1993) are all of interest for analysis of the spectrum of χ Lupi. An extensive analysis of Y II has been published (Nilsson *et al.* 1991).

Several references in this report are to papers presented at an international colloquium held in September 1992; additional reviews and presentations of atomic data of interest for astronomy will be found in the published proceedings (Leckrone and Sugar 1993).

B. Wavelength Standards.

The group at Imperial College has measured FTS spectra of an iron-neon hollow-cathode lamp and selected about 1100 Fe I and Fe II lines as recommended reference wavelengths in the range from 1830 Å to 4.25 μm . The most recent papers are by Nave *et al.* (1991, 1992); the 1991 paper gives wavelengths for 534 lines in the region 1830–3841 Å, with an uncertainty of 0.002 cm^{-1} (0.00008 to 0.00015 Å), and the 1992 paper has 290 lines from 4235 Å to 4.25 μm , with uncertainties of 0.001 to 0.0005 cm^{-1} .

Brault (1993) has measured the wavenumbers of selected Ar I lines excited in a low-pressure emission source with precision better than 0.00001 cm^{-1} . The absolute transition wavenumbers and energy-level values from this work will give new standards for FTS emission spectrometry in the 4170–14350 cm^{-1} region.

Users of ultraviolet reference lines from platinum-neon hollow-cathode lamps now have available an atlas of the spectrum from 1130–4330 Å (Sansone *et al.* 1992). The wavelengths of some 3000 of the 5600 lines included in an accompanying table are accurate to 0.0020 Å, with some of the Pt II Ritz-type wavelengths having uncertainties down to 0.0004 Å.

C. Compilations of Laboratory Data, Databases and Bibliographies.

Morton's (1991) compilation of data for 2031 resonance lines covers all spectra of hydrogen through germanium having allowed absorption transitions originating on ground-term levels with wavelengths longer than 911.75 Å. This compilation includes transition probabilities and other data, but is cited here because Morton tabulated the most accurate available wavelengths.

New compilations of wavelengths with energy-level classifications have been published for all spectra of magnesium, aluminum, and sulfur (Kaufman and Martin, 1991a, 1991b, 1993), and similar compilations for sodium and silicon are underway. The data are mainly based on earlier NIST compilations of the energy levels, but these are being updated and extended for many of the spectra to produce more accurate and complete wavelengths as calculated from the level values. A recent compilation of energy levels and wavelengths for O II has data based on newly optimized level values (Martin *et al.*, 1993). C. E. Moore's tables of energy levels and multiplets for hydrogen, carbon, nitrogen, and oxygen spectra, originally published during the period 1970–1985, have been collected into a single volume that includes data for O II based on the new compilation (Moore, 1993).

The most recent compilations by Shirai *et al.* of wavelengths and energy-level classifications for high ionization spectra of several elements ranging from vanadium to copper are also included in Table 1.

A fairly recent description of several of the larger and more inclusive collections of computer-readable atomic data (Martin 1992) need not be repeated here. As an addition, however, it may be noted that the library of computer-accessible data maintained by the Collaborative Computational Project No. 7 includes an extensive collection of atomic data (Jeffery 1993).

A biannual series of bulletins on atomic and molecular data for fusion includes references for recent papers with data on atomic energy levels and wavelengths (Botero 1992).

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WORKING GROUP 2: ATOMIC TRANSITION PROBABILITIES

W. L. Wiese, Chairperson

The Data Center on Atomic Transition Probabilities at the National Institute of Standards and Technology (NIST), formerly the National Bureau of Standards, in Gaithersburg, Maryland 20899, USA, is continuing its critical data compilation work and is also engaged in developing a comprehensive numerical database. In addition, the existing bibliographical database is continuously updated. The current compilation work concentrates on tabulating transition probabilities for allowed, as well as forbidden lines of light elements.

Extensive data tables for all ions of carbon, nitrogen, and oxygen are near completion. Work is also progressing on other light elements, specifically hydrogen, helium, lithium, beryllium, boron, fluorine, and neon.

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 XXIA, 111 (1991); preparation date: July, 1990) to the present (August 1993). 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: 40,53,106,121	Fe IV: 111	O I: 22,30,31,39,76,
Al II: 52,85,114	Fe VII: 107,108,109	94,116,117
Al III: 65	Fe VIII: 109,135	O II: 23,134
	Fe X: 64	O III: 5,6,16
Ar I: 81		O IV: 33
Ar II: 35	Ga I: 40	O V: 7,34,85,124
	Ga II: 52	O VI: 50,92
B II: 52,85		O VII: 43
B IV: 43	He I: 3,43,45,47,62,	
	113,120,122,128	P I: 96
Ba II: 55,102,123		
	Hg I: 95,106	Rb I: 13,74,123
Be I: 85	Hg II: 41,132	
Be II: 14,55	Hg III: 41	S I: 54,56,96
Be III: 43,85		S II: 78,134
	In II: 52	S III: 134
Bi I: 44		S V: 85
	K I: 74,88,97,135	
C I: 69,72,117		Si I: 96,98,133
C III: 7,8,17,85	Kr I: 81,106	Si II: 19,58,59,77
C IV: 17,37,50,92	Kr II: 35	Si III: 19,85
C V: 43,85,129		Si IV: 19
	Li I: 13,85,92,97	
Ca I: 85	Li II: 43,85	Sr I: 131
Ca II: 11,20,55,70,102,135		Sr II: 55,70,102,123
	Mg I: 9,18,28,48,63,	
Cd I: 106,127	79,84,85,106	Ti I: 89,90,103,105
Cd II: 20,88,126	Mg II: 55,88,93	Ti II: 110
		Ti IV: 135
Cl II: 134	N I: 21,25,26,67,68,	Ti VI: 64
	69,75,106,117	
Co I: 106	N II: 15,21,24,42,60,	Tl II: 52
	61,134	
Cr I: 106,115	N III: 33,80,82,83,119,130	Xe I: 81
Cr II: 1,112,115,118	N IV: 7,8,34,49,85,	
Cs I: 13,74,102,106,123	87,124	Zn I: 36,51,95
	N V: 14,50,85,86	Zn II: 20
Cu I: 2,27,106,125	N VI: 43	
F I: 38	Na I: 13,44,74,85,88,	
	93,97	
Fe I: 12,57,99,111,115		
Fe II: 4,10,29,57,71,	Ne I: 2,46,66,81,91,100	
73,101,104,111,115	Ne II: 32,35,38	
Fe III: 111	Ne III: 134	

Some outstanding developments in this field during the last three years have been: (a) the completion of the Opacity Project including the publication of several more papers summarizing the very extensive and sophisticated calculations of transition probabilities for various light element sequences [7,8,21,39,109,124]; (b) calculations of accurate transition probabilities with the configuration-interaction computer code CIV 3 by Hibbert and co-workers for neutral carbon, nitrogen and oxygen and some of their lower ions [5,23,24,75,119]; (c) very precise calculations for ions of the helium sequence [43], and (d) various very accurate measurements of atomic lifetimes [15-17,60,83,113] including those of levels that combine to the ground state only via intersystem lines [42].

The main part of this report is a bibliography containing 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 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 (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.

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WORKING GROUP 3. ATOMIC AND MOLECULAR COLLISIONS

J. W. Gallagher, Chairperson

A. ELECTRON COLLISIONS WITH ATOMS AND ATOMIC IONS

New general resources include Volume 32 of "Advances in Atomic, Molecular, and Optical Physics" edited by M. Inokuti [56], scheduled for publication in late 1993, which assesses the current status of collisional cross section data. It includes surveys of collisional cross-section data sources, but not extensive listings of data. The proceedings of the Third Atomic Data Workshop, held at Meudon Observatoire de Paris, September, 1989, provides a variety of useful reports [108].

An annotated bibliography by Itikawa [57] lists papers on experimental and theoretical studies of electron-impact excitation and ionization of atomic ions. A bibliography by Pradhan and Gallagher [90] reviews the quality of theoretical electron impact excitation papers.

The Iron Project, an outgrowth of the international Opacity Project, will provide high-accuracy calculated data for electron collisions with astrophysically prominent atoms and atomic ions. Specifically, the current

focus is the calculation of cross sections and rate coefficients for the fine structure transitions for infra-red spectral diagnostics, collisional data for all iron ions, and collisional and radiative data for the low ionization stages of iron (Fe I-VI), nickel and other iron-group elements. The status of this work is described in three new publications [55,65,109].

Important reviews by Cartwright et. al. [33] and by Trajmar et. al. [102] summarize and review data for electron impact excitation of helium. Another important article by Pradhan [88] reviews electron impact excitation for Fe I - Fe VIII. Many individual studies of electron-impact excitation of neutral atoms and atomic ions have been reported in the last three years and these are listed in Table 1. New studies of electron-impact ionization are listed in Table 2.

Table 1. References on electron impact excitation of neutral atoms and atomic ions.

H seq	38	O II	75	Si X	109
H I	68,69,3,34	O III	9,22,2	S I	110
H I	4,48,98	O IV	66,25	S II	54,32
He I	33,102,70,47	O V	60	S VII	81
He I	95,97,84,50	O VI	17	Cl IX	77
He I*	71	F IV	40	Ar I	28,29,24
He II	8	Ne I	28	Ar III	59
Li seq	111	Ne V	64	Ar VII	52
Li I	26	Ne VI	109	Ar VIII	17
Li II	19	Na I	82,23,27	Ar IX	80
Be seq	110	Na VI	40	Ar XIB	109
Be I	49	Mg I	39	Ca II	105,106
Be II	63	Mg II	63	Ca XV	5,6
Be ions	18	Mg IV	76	Ca XVI	109
B I	83	Mg VII	30	Ca XX	11
B ions	18	Mg VIII	109	Fe II	89,91
C II	66,25	Al III	82	Fe III	20
C IV	17,31	Al IX	109	Fe VII	61
C VI	10	Si II	45	Fe IX	46
N I	44	Si III	52	Fe XVII	21
N III	66,25,100	Si IV	17,104	Fe XXI	1
O I	62,58,72,103	Si VI	79,78	Fe XXVI	12

Table 2. Studies of electron-impact ionization.

He I	94	Ar I	74
C IV, N V, O VI	93,94	Ar III	67
O I	37	Ar VII	92,113
Ne VIII	41	Ar IX	125
Mg I	73	Ar XVI, Fe XXIV	112
Mg II	85	Ca II	15
Cl II	42	Fe ions	16
Si II, Si III	43	Kr ions	67,35,16,36
Si VII, Si VIII	107		

Progress has been made in dielectronic and radiative recombination, both experimentally and theoretically. Pequignot et al. present parametric fits for all H, He, C, N, and O ions [86].

Data references contain data in the form of cross sections, collision strengths, and/or rates. Each reference is annotated with a (T) theoretical; (E) experimental; (E/T) both.

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Rate Coefficients for Chemical Reactions (W. F. Huebner)

Chemical reactions, in particular their rate coefficients, are a form of atomic and molecular data that have not been reviewed by Commission 14 in the past. Chemical reactions can be categorized according to the phases of the reactants: (1) gas phase (neutral - neutral reactions), (2) plasma (ion - molecule reactions), (3) solutions, in particular non-ideal solutions (liquids and solids), and (4) heterogeneous or catalytic reactions (usually gas - solid). Catalytic reactions in which the third body is a gas are usually listed under gas-phase reactions. In astrochemistry, gas-phase reactions are of prime interest in modeling cold dense systems such as planetary atmospheres (Levine, 1985), protostars, the solar nebula, and preplanetary subnebulae (Howe et al., 1992). Plasma or ion - molecule reactions are of interest in circumstellar envelopes (Glassgold et al., 1992), the interstellar medium including diffuse (van Dishoeck, 1990) and dense clouds (Hasegawa et al., 1992), the solar nebula, ionospheres of planets and satellites, and comet comae (Schmidt et al., 1988).

This first review of rate coefficients for chemical reactions centers on basic definitions to guide potential users and introduce them to existing databases.

Chemical kinetics deals with the time rate of chemical change and with the use of measured and calculated rates to explain and clarify the mechanisms by which chemical systems approach thermodynamic equilibrium or a steady state. A complication arises when a reaction proceeds through a *kinetically stable* (i.e., thermodynamically metastable) state which is separated from the *thermodynamically stable* state by a potential energy barrier and the reaction energy is insufficient to overcome the barrier. In this case, true chemical (thermodynamic) equilibrium may be reached only after an infinite time.

Chemical reactions depend on the concentration of the reactants and the speed of the reactions, i.e., the rate coefficients. The species concentrations depend also on the rate of the gas flowing through the reaction volume. The rate of a chemical reaction can be described by

$$\partial n_i / \partial t = P_i - L_i - \nabla \cdot \mathbf{v}_i n_i, \quad (1)$$

where n_i is the concentration (number density) of a product species i , P_i and L_i are the chemical production and loss terms for species i , and the last term in Eq. (1) is the divergence of the flux of particles having velocity \mathbf{v}_i . It is this last term which may prevent reactions from reaching equilibrium. The rates of most chemical reactions increase rapidly with increasing temperature. The rate coefficient data measured or calculated at temperature T are normally fitted to the standard Arrhenius form for collisional processes

$$k = A (T/300)^B \exp(-C/T). \quad (2)$$

Here T is either the gas, ion, or electron temperature depending on the physical process. The dimensions of the A coefficient contain concentrations for all except the first-order reactions (e.g., photo reactions). The coefficient C contains the activation energy. The rate coefficient k is independent of concentration of the reactants, but may depend strongly on temperature.

Rate coefficients for a forward (exothermic) reaction and its reverse (endothermic) reaction are related by the equilibrium coefficient

$$K = k_r / k_f \quad (3)$$

Equilibrium coefficients as a function of temperature and relative to reference states are given in the JANAF Thermochemical Tables (Chase et al., 1985). Additional information about the relationship of rate coefficients, equilibrium coefficients, and thermodynamic variables can be found in Cohen and Westberg (1983, 1991).

Databases for chemical reaction networks are available in several formats. The NIST (National Institute of Standards and Technology) database (Mallard et al., 1993) contains measured data, means of entering additional data, and computer codes for analyzing and fitting data to an Arrhenius equation. The data in the current version (5.0) include reactions for 6400 distinct reactant pairs in thermal gas-phase kinetics, particularly for combustion, i.e., hydrocarbon chemistry. The least squares fit Arrhenius parameters (A , B , and C in Eq. 3) can be saved to a file together with the reaction species (reactants and products) and the temperature limits for the data fit. The NIST Chemical Kinetics Database provides a powerful and flexible tool, but requires manipulative effort on a PC.

Ion - molecule gas phase reactions have been compiled by Anicich (1993). The compilation includes rate coefficients for reactions of the first 30 elements in the periodic table (except Li and Be) plus bromine, krypton, zirconium, silver, xenon, and barium for quoted temperatures, usually around 300 K. Certain classes of ion - molecule reactions are not sensitive to temperature and can thus be presented by a single parameter. Another compilation of rate coefficients for astrophysical and planetary applications is the UMIST rate file (Millar et al., 1991). The latest version (UMIST Database for Astrochemistry Rate 92) contains about 390 chemical species and over 3700 reactions. Rate coefficients for astrochemistry in general have been published by Millar and Williams (1988).

Reaction rates for aeronomy were discussed by Fox (1991). Solar photo rate coefficients for dissociation, ionization, and dissociative ionization have been calculated and evaluated on a uniform basis for about 100 atomic and molecular species (Huebner et al., 1992).

Finally, for calculating rate coefficients for reverse reactions, tables of equilibrium coefficients have been compiled on a uniform basis at temperatures up to 6000 K in the JANAF Thermochemical Tables by Chase et al. (1985). Equilibrium coefficients have been incorporated in the NIST Chemical Kinetics Database and are also available on magnetic tape from NIST. In addition, the equilibrium coefficients are useful to determine astrophysical chemical equilibrium compositions including condensation sequences, as for example, in the solar nebula (Sharp and Huebner, 1990).

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WORKING GROUP 4 : LINE BROADENING

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The field of line broadening has continued to be very active during the last three years, mostly stimulated by the interpretation of recent observations or by the preparation of space investigations. It is not the aim of this report to be exhaustive, so we will simply give a number of useful results for astrophysical purposes.

We will mention an important and very useful Bibliography on Atomic Line Shapes and Shifts (1), jointly established by the Département d'Astrophysique Stellaire et Galactique of the Observatoire de Paris-Meudon (A. Lesage) and by the NIST Data Center (J. Fuhr). This important piece of work is concerned with Stark broadening and shifts as well as Van der Waals broadening and covers the literature from July 1978 to March 1992. Concerning these topics, the present report is mainly confined to a selection of references on the basis of their astrophysical interest.

1. Stark Broadening

1.1 STARK BROADENING FOR PLASMAS OF LOW DENSITIES: THE IMPACT LIMIT

First considering low to moderately dense plasmas, the Opacity Project constitutes a major effort to produce extensive calculations of atomic data required for opacity determination. This work includes Stark broadening of atomic and ionic lines. For atoms (except H) and non hydrogenic ions, the dominant contribution to the broadening is due to electronic collisions. Use of the R-Matrix method leads to very accurate results for transitions involving states of low excitation, and approximate formulae have been developed for transitions between higher excited states.

Approximate methods (semiclassical perturbation theory) have been used extensively by several groups to provide broadening parameters for a large number of lines of astrophysical interest, with a mean accuracy of about 20 to 30 percent. Furthermore, much work has been done experimentally.

Table 1 presents references containing 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 number of the reference list.

Another interesting and complementary direction concerns investigations of systematic trends of Stark broadening parameters. Regularities of these parameters within a multiplet or within spectral series and homologous atoms have been investigated (6, 21, 32-34).

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

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 when the emitter is either the H atom or an hydrogenic ion. The quasistatic approximation used for ionic broadening at low densities is no longer valid in these cases. Simultaneous strong interactions between the radiator and the surrounding ions may occur. The relatively high velocities of the perturbers preclude the consideration of these interactions as static and much effort, both experimental (36-39) and theoretical (10, 40-44), has been devoted these last

Table 1.

Ar I	2	Cd II	12	O I	25
Ar III	3			O II	26
Ar IV	3,4	F I	6		
		F II	13	S II	3,27
B I	5	F III	13	S III	27
B II	5				
B III	5	He I	14,15,16,17		
				Si II	28
Br I	6	Hg I	18,19	Si III	22,29
Br II	7	Hg II	18	Si IV	29,30
Br III	7				
Br IV	7	Li I	20	Xe I	31
				Xe II	31,32
C I	2,8	N II	21		
C II	8	N IV	22		
C IV	9,10	N V	22,23		
Ca II	11	Na I	5,24		

years to this many body dynamical problem. The physical limit between bound and free states becomes a function of the density and the temperature, leading to the disappearance of higher spectral series numbers. Such studies lead to interesting improvements of the Inglis Teller formula. Consequences for the determination of opacities have been analyzed (45). In the infrared, a correct modeling of the broadening of the solar hydrogen lines (46) gives profiles in a generally good agreement with the observational data of ATMOS.

2. Line Broadening by foreign gases and molecular line broadening

2.1 BROADENING OF ATOMIC LINES

Pressure broadening of neon (47), argon (48) and caesium (49) lines by various rare gases has been investigated experimentally. Many calculations involving various degrees of sophistication in the determination of interatomic interactions have appeared in the literature: self broadening of helium lines (50), Ca lines perturbed by H (51), alkali resonance lines perturbed by H and rare gases (52). One has to mention interesting results on the broadening of Rb Rydberg lines by rare gases (53).

2.2 FAR WINGS

Far wing profiles have received less attention. New data are available on Ba (54, 55) and Ar, Kr, Xe perturbed by Ne (56, 57). The temperature and density dependence of the Lyman α line wing in hydrogen-rich white dwarf atmospheres have been investigated (58).

2.3 MOLECULAR BROADENING

Concerning pressure broadening of molecular lines, many important results have been obtained; for astrophysical purposes we will quote particularly the calculation of the broadening parameters of CO (59), HD perturbed by He and H₂ (60), and line width measurements in H₂O (61, 62). Many theoretical or experimental investigations in this domain have been greatly stimulated by new spatial observations of planetary atmospheres: particular attention has been given to collisional broadening of C₂H₄ (63), C₂H₂ (64), CD₄ (65), NH₃ (66, 67), CH₄ (68,69). Very important results were reported on CO₂(70-73).

A special attention has been paid to the difficult problem of line mixing in CO₂ (74), CO and CO₂ (75), HCN and C₂H₂ (76). This considerable effort in molecular line broadening has contributed to the improvement of molecular databases (HITRAN (77), 1991GEISA (78)) which provide the necessary fundamental parameters to represent molecular properties in atmospheric spectroscopic analysis. Although focussed on terrestrial atmospheric studies, many of the listed data are very important for outer planets.

2.4 COLLISION INDUCED SPECTRA

Collision induced absorption is known to be the main source of opacity of the outer planets, which are composed of non polar molecules like hydrogen and helium. Recently a new interest for collision induced spectra has appeared with the need of molecular opacities for the modeling of cool and dense stars: white dwarfs, brown dwarfs, protostars...

Accurate calculations of collision-induced infrared absorption spectra of H₂-H₂ and H₂-He pairs (79-82) have been carried out. The agreement between the theoretical model and the experimental data is usually good to within a few percent, except for the H₂-He spectra calculated at 296 K which does not agree with the latest measurements (83). The reason for this discrepancy is still unsolved. New measurements of the collision induced emission in H₂-H₂, Ne, Ar, Xe are available (84). Calculations of the far infrared spectra of N₂-CH₄ pairs are presented in (85). This work is of interest for the modeling of Titan's atmosphere.

Collisional interference between electric dipole allowed and collision induced transitions has been investigated (86).

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WORKING GROUP 5: MOLECULAR STRUCTURE AND TRANSITION DATA

W. H. Parkinson, Chairperson

This report has been compiled in large part from edited contributions sent to me in the summer of 1993.

Laboratory and theoretical studies in molecular spectroscopy and the resulting molecular data and parameters have continued to grow with the needs of chemists, physicists and astronomers. The number and holdings of atomic and molecular databases,^{1,2,3} have increased. The expansion and inclusion of atomic and molecular data (AMD) on the interactive, rational database, Astrophysical Data System (ADS) will soon begin at the Harvard-Smithsonian Center for Astrophysics (CfA). Information about AMD in ADS is available from Peter L. Smith. The useful molecular bibliography, Berkeley Newsletter, continues to be available from Davis and colleagues.

The period 1990-1993 could be remembered for the basic spectroscopic studies of H_3^+ and for the use of its infrared spectrum as an astronomical probe.⁴ The infrared H_3^+ emission of the ν_2 fundamental band has been established as a powerful ground based observational tool to study plasma activities in planetary ionospheres. H_3^+ spectra have been observed in the Jovian atmosphere^{5,6,7,8,9} and in the atmospheres of Uranus¹⁰ and Saturn.¹¹ Recent improvements in spectrometer sensitivity are expected to lead to detection of H_3^+ in Neptune.

Takeshi Oka has reviewed the indispensable, close collaboration of astronomers, laboratory spectroscopists, and theorists for the study of H_3^+ . The H_3^+ spectrum of hot bands $2\nu_2(2) \leftarrow \nu_2$, $2\nu_2(0) \leftarrow \nu_2$, and $\nu_1 + \nu_2 \leftarrow \nu_2$ have been reported¹² along with laboratory measurements of the first overtone band¹³ $2\nu_2(2) \leftarrow 0$ and the second overtone band¹⁴ $3\nu_2(1) \leftarrow 0$. Rotational levels up to $J=K=15$, 5092 cm^{-1} above the $J=0$ state, have been observed and the data have been summarized.¹⁵ Forbidden transitions $\nu_1 \leftarrow 0$, $\nu_1 + \nu_2 \leftarrow \nu_2$ have been observed.¹⁶ The ν_2 fundamental band of H_3^+ has now been observed in absorption by using a Fourier transform spectrometer (FTS).¹⁷

Basic theoretical calculation^{18,19,20} of the vibration-rotation levels of H_3^+ played a crucial role in the identification of the laboratory spectrum and the Jupiter emission spectrum. The theory has been extended to forbidden²¹ and overtone²² transitions. Recently, Watson²³ has modified the *ab initio* potential of Meyer, Botschwina, and Burton by a least squares procedure to fit the observed frequencies. A new *ab initio* calculation of the potential has been given by Frye and others^{24,25}, and the potential recently modified²⁶ to fit the observed frequencies and predicted higher vibration rotation states.

The very large discrepancy in values of the H_3^+ electron recombination rate seems to have been settled by laboratory measurements. Amano²⁷ published details of his earlier spectroscopic experiment and concluded that the recombination rate is $1.8 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$ at 273 K. A flowing after glow/Langmuir probe experiment²⁸ gives $1.1 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$ at 650 K. The rate below 1 eV of vibrationally cooled H_3^+ is $6 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$ from measurements²⁹ made at the ion storage ring, Manne Siegbahn Institute of Physics, Sweden and is in satisfactory agreement with the merged-beam experimental value³⁰ of $2 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$.

A. R. McKellar has reported results from the Herzberg Institute of Astrophysics. Among diatomic molecules, electronic spectra have been studied for N_2 ,^{31,32} O_2 ,³³ OH ,³⁴ and NO^+ .³⁵ In the infrared region, work on the spectra of weakly-bound dimers include experiments on the H_2 dimer^{36,37} and the NO dimer³⁸. A new technique involving high resolution infrared detection has been applied to measuring dissociative recombination rates for the ions H_3^+ , HN_2^+ , and HCO^+ .²⁶ In addition to these molecular ions, a number of other unstable polyatomics have been studied in various wavelength regions. These include infrared³⁹ and vibration-rotation⁴⁰ spectra of NH_2 , a near-infrared electronic spectrum of triplet C_3 ,⁴¹ vibration-rotation spectra of C_2D ⁴² and $^{13}C_3$,⁴³ and pure rotational spectra of NCS ⁴⁴ and $HCCCO$.⁴⁵ Work has continued on the precise measurement of infrared intensities of CO_2 .^{46,47} A large number of stable polyatomic molecules have been studied at high resolution in the infrared region, including H_2O_2 ,⁴⁸ ketene,⁴⁹ acetaldehyde,⁵⁰ $HNCO$,⁵¹ $OCCCS$,⁵² C_2H_2 ,⁵³ C_2H_6 ,⁵⁴ C_4H_2 ,⁵⁵ C_6H_6 ,⁵⁶ CH_3OH ,⁵⁷ C_3O_2 ,⁵⁸ and DNO_3 .⁵⁹

Investigators at the CfA have reported studies of fundamental molecular parameters and processes. Basic calculations have been carried out by K. Kirby and colleagues⁶⁰ of all the potential curves and transition moments relevant to the photodissociation of HCl^+ and the charge transfer of $H^+ + Cl$. Direct photodissociation cross sections, transition moments, and radiative lifetimes of NH have been computed by Kirby and Goldfield.⁶¹

The millimeter-wave and far infrared spectra of $HOCO$ and $DOCO$ have been detected in the gas phase and studied in the CfA laboratory.^{62,63} In combination, the investigations yield a complete set of precise spectroscopic constants for the molecules. Quantitative studies at high wavelength resolution of molecules of atmospheric importance have been continued by Yoshino and colleagues. Predissociation linewidths of the O_2 Schumann-Runge (S-R) bands have been obtained from the high resolution cross section measurements of the isotopes, $^{16}O_2$,⁶⁴ $^{16}O^{18}O$,⁶⁵ and $^{18}O_2$.⁶⁵ Theoretical studies of the predissociation of the S-R bands and their rotational dependency have been carried out.^{66,67} Cross sections in regions of the transmission windows of the S-R bands have been obtained along with the weak Herzberg continuum cross sections under the S-R bands.⁶⁸ The oscillator strengths of the hot bands (from $v' = 1$) of S-R system have been obtained.⁶⁹ Polynomial coefficients for calculating the S-R cross sections have been determined⁷⁰ and the results agree with the high resolution measurements over the temperature range 78 K to 570 K. The absolute cross sections of ozone have been obtained⁷¹ in the wavelength region 185-254 nm at temperature, 295 K, 228 K, and 195 K. No temperature dependency is observed. The solution to the need for absorption measurements at higher wavelength resolution has been pursued by Yoshino and colleagues with the vacuum UV FTS at Imperial College, London, England. Measurements have been completed at a resolution of 0.06 cm^{-1} of absorption cross sections and band oscillator strengths of the $\delta(0,0)$, $\delta(1,0)$, and $\beta(7,0)$ bands of NO . Work is also underway to measure the absorption cross sections of the O_2 Herzberg I band system ($A\ ^3\Sigma_u^+ - X\ ^3\Sigma_g^-$) at a resolution of 0.06 cm^{-1} with the FTS in combination with a White cell. A number of other high resolution measurements of VUV molecular cross sections have been made: C_2H_2 , 147-201 nm,⁷² CO , $E(0,1) - X(0)$,⁷³ N_2 , 95.5-100 nm,⁷⁴ and CO between 96.7 and 98.8 nm at 20 K.⁷⁵ The work includes the first supersonic jet-cooled absorption cross section measurement on molecules cooled to about 30 K. Additional absorption cross section data (CO 92.5-96 nm @ 30 K and HCl C-X bands) will soon be available. Adjunct studies of CO at CfA and independently by Ubachs⁷⁶ disclosed a small systematic error in published wavelengths/wavenumbers for CO ,^{77,78} Eidelsberg *et al.*⁷⁹ discuss the recalibration.

C. E. Brion and colleagues have recently applied the electron-impact (EI), dipole (e,e) excitation method⁸⁰ to the measurement of absolute oscillator strengths for transitions in H_2 ,⁸¹ N_2 ,⁸² O_2 ,⁸³ NO ⁸⁴ and CO .⁸⁵ The method appears to have some advantages over direct optical measurements and over other EI experiments. When results are compared, there are both satisfactory agreements^{86,74} and puzzling discrepancies.^{73,87}

Theoretical calculations of optical and generalized oscillator strengths for relevant transitions in CO have been carried out by R. E. Buenker and colleagues.^{88,89}

P. K. Carroll at University College, Dublin has reported the measurement and analysis of the $^1\Sigma_u^+$ states of N_2 ¹⁵ from high resolution absorption spectra in the 89.5-77.0 nm region.⁹⁰

F. Rostas has outlined the activities in molecular research of the Meudon group. These include a new determination of the ground state potential of N_2 ⁹¹ and the vibrational analysis⁹² of low pressure emission spectra of N_2 between 107.7 and 124.7 nm. An atlas of the EUV absorption spectrum of CO ^{77,79} has been published as well as band-integrated optical absorption cross sections for the $A\ ^1\Pi(v-12) - X\ ^1\Sigma^+(v)$ transitions.⁹³ Studies of the photodissociation process involving the $CO\ B\ ^1\Sigma^+ - D\ ^1\Sigma^+$ interaction,⁹⁴ a two photon study of the $E\ ^1\Pi$ state⁹⁵ and an analysis of the perturbation of the $D\ ^1\Delta$ state,^{96,97} have been published. The constants of the $X\ ^1\Sigma^+$ state of CO have been improved.⁹⁸ Line positions and emission probabilities of the Lyman and Werner band systems have been calculated taking into account the interactions of the B, B', C and D states.^{99,100} Nine rotationally resolved bands of CO_2 have been analyzed¹⁰¹ and *ab initio* calculations support the analysis.¹⁰² Low lying linear Rydberg states have also been calculated, providing a model for the CO_2 "Rathenau bands" in the 11.4-12.6 eV range¹⁰³ and Rydberg-valence interactions for the lowest lying Rydberg states around 11 eV.¹⁰⁴ The vibration-rotation spectrum of Si_2C ¹⁰⁵ and $CO_2^+(X\ ^2\Pi_g)$ ¹⁰⁶ have been calculated. The electronic spectrum of Fullerenes has been recorded between 190 and 750 nm and analyzed in terms of Herzberg-Teller couplings;^{107,108} triplet-triplet transitions have been observed in pulsed experiments.¹⁰⁹

R. W. Nicholls (Center for Research in Earth and Space Science, York University) reports on new NbO bands¹¹⁰ from shock excitation of powered Nb_2O_5 . A theoretical basis for an extended Birge-Mecke rule of molecular spectroscopy,¹¹¹ augmented sum rules for progressions of Franck-Condon factors for bound-free and free-free transitions,¹¹² and new line parameters for the O_2 Herzberg I system,¹¹³ have been obtained. A new identification atlas of the atmospheric and infrared atmospheric band system of O_2 is available from Nicholls.

Franck-Condon factors and the r-centroids for the bands $A^2\Pi - ^2\Sigma^+$ of CP , $C^3\Pi - X^3\Pi$ of SiC , and $B^2\Sigma^+ - X^2\Sigma^+$ of CO^+ , and potential energy curves and dissociation energies of NbO , SiC , CP , PH^+ , SiF^+ , and NH^+ have been published by Reddy and colleagues.^{114,115}

Sumner Davis and John Phillips have reported on a variety of important molecular spectra. They have observed and measured highly excited rotational states of the OH Meinel band system,¹¹⁶ as produced in a N_2 -afterglow. These results were incorporated into a theoretical study.¹¹⁷ Davis and colleagues¹¹⁸ have extended measurements on the $OD(1,0)$ band and measured the $(2,0)$ band for the first time. A CN spectrum¹¹⁹ from 9000 to 31,000 cm^{-1} was recorded in a N_2 -afterglow containing a trace of CH_4 ; the data contain C^{12} and C^{13} . Work on the iron hydride spectrum has continued with the band in the 700 nm region considered to be $HFeH$.¹²⁰ The quartet and sextet states of FeH have been studied theoretically by Langhoff and Bauschlicher.¹²¹ The calculations are entirely consistent with the earlier observations of the near-infrared system by Phillips and Davis, but the spectroscopic designation should be $F\ ^4\Delta - X\ ^4\Delta$. Theoretical studies of FeH^+ have also been presented by Langhoff and colleagues.¹²² Earlier work by Littleton and Davis¹²³ on transition strengths in the singlet and triplet systems of ZrO as measured from emission spectra was inconsistent with stellar data and did not agree with the calculations of Langhoff and Bauschlicher.¹²⁴ New absorption spectra have been analyzed.¹²⁵ A synthetic spectrum, calculated with the new parameters, matches the observed spectrum and removes inconsistencies. Langhoff and colleagues¹²⁶ have studied the Phillips band system of C_2 and have calculated the radiative lifetime of the $A\ ^1\Pi_u$ state ($v' = 0, J' = 1$); these calculations suggest a large systematic error is possible in the measurements of Bauer *et al.*¹²⁷ The line strengths for the ro-vibrational bands of $X^1\Sigma^+$ state of SiO have been calculated by Langhoff & Bauschlicher.¹²⁸

U. G. Jorgensen has computed the line strengths for 4×10^6 lines of the $A\ ^2\Pi - X\ ^2\Sigma^+$ Red system of CN .¹²⁹ Line lists for TiO , CH , H_2O , and HCN are under construction and a review of existing astrophysical molecular data has been published.¹³⁰ A complete and very accurate computation of the 8×10^4 existing vibrational transitions in the H_2O ground electronic state is in press.¹³¹

Michael E. Mickelson, Denison University, Ohio, has described measurements of the absorption coefficient for the 619 nm visible CH_4 band between 300 K -150 K.^{132,133} A new cold absorption cell and a tunable dye laser (linewidth 0.06 cm^{-1}) are used. Molecular parameters for H_2 , including line positions, strengths, pressure-broadening coefficients and shifts, have also been determined^{134,135} from measurements with a long

path absorption cell (2-6 Km) and a spectrometer (resolution $.015 \text{ cm}^{-1}$) or tunable dye laser (resolution $3 \times 10^{-5} \text{ cm}^{-1}$).

Frank J. Lovas has published¹³⁶ a new revision to the 1985 edition of the recommended rest frequencies for observed, interstellar molecular microwave transitions. He and colleagues have measured low-J rotational transitions¹³⁷ in SO, C₂S, C₃S, c-HC₃, CH₂CC and c-C₃H₂. The frequencies measured are sufficient to allow molecular dynamics of cold interstellar clouds to be determined with improved accuracy. Molecular electric dipole moments have also been determined for SO, C₃S, c-HC₃ and c-C₃H₂. New measurements and analysis of the ν_5 and $2\nu_9$ infrared absorption bands of HNO₃ have been made;¹³⁸ in the range 850 cm^{-1} - 920 cm^{-1} , the bands are important in the spectrum of the Earth's upper atmosphere.

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WORKING GROUP 6: MOLECULAR REACTIONS ON SOLID SURFACES

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Molecular reactions on solid surfaces is a new subject for a report to Commission 14. From the astrophysical viewpoint it concerns the physical chemistry of dust and grains. These entities are chemically active, the major illustration of which is the association of hydrogen atoms at interstellar dust surfaces to form molecular hydrogen. Observations of H₂ in diffuse clouds imply that this is an efficient process. Several other recent observations of interstellar molecular abundances appear to be incompatible with purely gas phase reactions, so that the intervention of grain chemistry is surmised. Development of this subject is hampered by the relatively small amount of knowledge we have as to the nature and composition of interstellar and solar system grains, and the structure and properties of the gas-grain interface. This makes it hard to evaluate key parameters such as sticking coefficients and adsorption, condensation, desorption and evaporation properties, as well as the thermal, photochemical and ionizing-radiation induced chemical reactions occurring on the surfaces and which can all contribute to gas-grain exchange. The present non-exhaustive report is intended to give some key indications to the physico-chemical background, model experimental and theoretical studies and to the astrophysical aspects of the subject.

1. Reviews

1.1. Reviews on the nature and properties of dust and on material processing in space.

Laboratory, observational and theoretical studies of interstellar ices (1); Models of interstellar grains (2); Ion-solid interactions (3); Meteoritic, interplanetary and cometary dust (4); Irradiation of solids (5); Mass-spectrometric in situ analysis of solid-state extraterrestrial samples (6); Spectroscopy of solid materials simulating cosmic dust (7); Molecule formation by fast particles in astronomical objects (8); Nucleation and growth of solid particles from high-temperature gas mixtures (9); Spectroscopy of ion-irradiated carbonaceous materials (10); Theory of Cosmic Grains (11); Observations and Theories of Interstellar Dust (12); Dust and its Chemistry in Astronomy (13-15).

1.2. Reviews on Surface Science.

Surveys of concepts and experimental techniques in surface chemical physics (16-19). Discussion on the Structure of Surfaces and Interfaces as studied using Synchrotron Radiation (20). Photochemistry and Radiation chemistry of Adsorbed Molecules (21)

2. Studies of Dust Grain Properties and Models.

Dust grain properties in Reflection Nebulae (22); Dust grain processing in the Orion nebula (23); Electric charge on grains in diffuse clouds (24); Dust coagulation (25); Dust grain composition, size and processing models (22-31). Cosmic -ray induced desorption (32); Carbon dust formation on interstellar grains (33). Hydrogenated Amorphous Carbon Grains and Mantles in the ISM (34-37).

3. Astrophysical observations and models suggesting molecule formation or gas-grain exchange.

NH in diffuse clouds (38, 39); H₂CO in exterior parts of dense clouds (40); D₂CO observations (41); Astrophysical models involving adsorption and chemistry on grains (42-48); Return or freezing out of gas material in the ISM(49-51); Chemical activity of dust (52-54).

4. Models of the Formation of H₂ on Dust Grains and its Excitation

Formation processes and possibility of observing infrared emission from H₂ formed on surfaces (55); ortho:para H₂ ratio (56); H₂ rotational level distribution (57); possibility of detecting H₂ on interstellar dust by infrared absorption (58).

5. Laboratory studies of hydrogen recombination and hydrogenation reactions on carbonaceous and on analogous materials.

Surface diffusion of hydrogen atoms on a silicon surface (59); Hydrogen-surface interactions (60); Chemical erosion of graphite by hydrogen atoms (61); Hydrogen atom chemisorption on a graphite surface (62); energetics of hydrogenated surfaces of diamond (63); Light-enhanced hydrogen motion in hydrogenated amorphous silicon (64); Hydrogen recombinative desorption on silicon and other surfaces (65-69).

6. Surface Properties and Dynamics.

Surface melting and role of surfaces in melting (70-72); Dynamics at Surfaces (73); Vibrations and Sticking of a particle on a Surface (74); Direct Observation of Chemical Bond dynamics on Surfaces (75); Hydrogen atom site-to site hopping rates (76); Heat capacities of physisorbed films on graphite (77); Experimental and theoretical studies of NH₃ adsorbed on graphite (78-81); Mechanisms and energetics of photofragmentation of molecules condensed on surfaces (82,83); Oxidation on carbon surfaces (84); Photon-induced Desorption of Molecules from Surfaces (85-87).

7. Laboratory Studies of Astrophysical-type Ices

CO₂ in astrophysical ice analogs (88); Clathrate hydrate formation in amorphous cometary ice analogs (89); H₂CO and organic molecule production in astrophysical ices (90); Condensation and structure of amorphous ice (91); Amorphization of cubic ice by UV irradiation (92).

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