

14. FUNDAMENTAL SPECTROSCOPIC DATA
(DONNEES SPECTROSCOPIQUES FONDAMENTALES)

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GENERAL

The title of our Commission was last changed in 1964 from "Commission des Etalons de Longueur d'Onde et des Tables de Spectres" to the present title recognizing the broader scope of the Commission. This was initiated by new observing techniques and refined theoretical models. In 1966 it was decided to add two more objects to the work of the Commission: Broadening of spectral lines and collision cross sections. The present structure of the Commission dates back to 1970. Since then the work of the Commission is not well described by the name "Fundamental Spectroscopic Data". This is a hindrance in the recruitment of new members, especially those who represent new fields of interest. But the answers to an enquiry about change of name were so divergent within our Commission that so far no action was taken.

Another problem in this context is perhaps more basic. For a certain time Commission 14 took up new fields of physics as the interpretation of new observations demanded. This does not seem possible any more. Needed fields not dealt with by Commission 14 are e.g. dust chemistry, atoms in high magnetic fields, extreme density matter and nuclear physics. On the other hand fields dealt with by Commission 14 are worked on by so many physicists that it is hardly possible to write a report on their work within the given limit of space. Many workers in these fields, even if they work especially for astrophysics don't even know that Commission 14 exists. Question: Do we serve our purpose best with the present structure?

E. TREFFTZ

WORKING GROUP 1: WAVELENGTH STANDARDS

The Primary Standard and the Velocity of Light

The situation as regards the primary standard has changed little since the last Commission 14 report in 1975 (1); it may be summarized briefly as follows: the International Metre is officially based on the 0.606 μm wavelength of ^{86}Kr , reproducible to about $\pm 1 \times 10^{-9}$. More reproducible wavelengths emitted by lasers stabilized on absorption lines of I_2 , CH_4 and CO_2 are known in terms of the Metre to about the same uncertainty ($\pm 1 \times 10^{-9}$) and can be considered practically equivalent to the primary standard. The frequencies of the CH_4 and CO_2 stabilized lasers are known in terms of the Cs primary standard of frequency to better than 10^{-9} . The resulting calculated value for the velocity of light ($c = 299792458 \text{ m/s}$) has been adopted as the best value by the International Committee of Weights and Measures, with the recommendation that in any future redefinition of the Metre, or of the second, this value should be unchanged and should be considered as exact. Thus the Metre can be considered as unofficially defined in terms of the velocity of light and the second. It was decided that it would be premature to propose an official redefinition of the Metre at the General Conference of Weights and Measures in 1979, but sufficient confirmation of the above value of c can reasonably be expected in time to make possible an official redefinition in terms of the Cs standard and an adopted value for c , at the General Conference in 1982. A number of stabilized laser systems are being investigated that are potentially more precise than the Cs standard but it is unlikely that they could be proven to be

better in time to satisfy the demand for a redefinition of the Metre. In the mean-time frequency comparison chains are being developed at a number of National Laboratories that will provide sources of radiation in the optical region, phase locked to the Cs frequency standard, and therefore accurate to $\sim 10^{-13}$.

The Rydberg

An improved measurement of the Rydberg has been made by Hansch and his colleagues at Stanford in the U.S.A. by the use of polarization spectroscopy of the $3^2P_{1/2} - 2^2S_{1/2}$ line of Hydrogen (2). They obtained the value $R_\infty = 109737.31476(32)$ cm^{-1} . Petley and Morris at N.P.L., England, have also made new measurements (3), finding $R_\infty = 109737.3167(15)$ cm^{-1} , based on $3^2D_{5/2} - 2^2P_{3/2}$ and $R = 109737.3179(15)$ cm^{-1} based on $3^2D_{3/2} - 2^2P_{1/2}$ of Hydrogen.

Secondary Standards

In addition to the standards provided by lasers stabilized on absorption lines of I_2 , CH_4 and CO_2 , mentioned above, radiations of comparable frequency reproducibility are produced by means of an Argon laser stabilized on I_2 at 515 nm and a CO_2 laser stabilized on lines of SF_6 or OsO_4 at 10 μm , but precise values for the wavelengths or frequencies have not yet been published. A He-Ne laser stabilized on an I_2 line at 612 nm has been measured at B.I.P.M., Paris, yielding a value for the wavelength $\lambda_{\text{vac}} = 611970458.6(.2)$ fm (4). Laser sources such as these are becoming of increasing importance as references for the control of automatic wavelength measuring interferometers. Of the relatively little recent work on thermal sources of wavelength standards, the following is noteworthy: Norlén and Johansson at Lund in Sweden have determined accurate values ($\pm 0.001\text{\AA}$) of 300 Fe II lines between 2380 and 3000 \AA (5). Freeman and his group at N.P.L., England, are continuing work on U.V. lines of Cu II, measuring shifts, line widths and suitability for standards, but have not reported precise wavelength values. An atlas of 22,850 lines in the visible absorption spectrum of the I_2 molecule has been produced at the Aimé-Cotton Laboratory in Paris (6). Internal consistency of ± 0.001 cm^{-1} and absolute accuracy of ± 0.006 cm^{-1} are given. Tables of standard wave numbers for infrared spectroscopy have recently been published through the initiative of the Inter-Union Commission on Spectroscopy (7). A review article on Wavelength Standards will be included in Part B of Progress in Atomic Spectroscopy, soon to be published by Plenum Publishing Co.

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K.M. BAIRD

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WORKING GROUP 2: ATOMIC TRANSITION PROBABILITIES

The Data Center on Atomic Transition Probabilities at the National Bureau of Standards, Washington, D.C., has continued its bibliographical and critical compilation work on transition probabilities. A new general bibliography has been

published, covering the literature references through October 1977 (1). It contains approximately 2400 references in chronological order and includes listings by element, stage of ionization, and experimental or theoretical method applied, as well as an author index. A critical compilation has been completed for V, Cr, and Mn (2), which covers all stages of ionization on which reliable data are available. Work is now in progress on Fe, Co, and Ni. A special NBS study has been devoted to oscillator strength distributions in various spectral series of Li-like ions (3), and from this work extensive tables of critically evaluated oscillator strengths for the Li sequence up to Ni XXVI have been derived (4). A number of reviews on calculations and measurements of atomic transition probabilities and lifetimes have recently been published. The books "Beam-Foil Spectroscopy", edited by S. Bashkin (5) and "Progress in Atomic Spectroscopy", edited by W. Hanle and H. Kleinpoppen (6) contain several chapters on these topics. About 500 theoretical and experimental papers containing data on atomic transition probabilities have been published since 1976. Thus, rather than aim for completeness, a general review of the progress is given, and a large number of representative papers are briefly discussed. The review of the theoretical work is divided into two parts: First, papers which are included in the above cited general NBS bibliography are discussed without citation. Later on, the more recent papers are quoted with full references.

A number of the recent papers include data and/or formulae for many ions of a given isoelectronic sequence and as such are of interest in photospheric and coronal studies. Lin, Johnson, and Dalgarno (1977) have used the relativistic random-phase approximation to calculate transition probabilities for radiative decay from $n = 2$ states of He-like ions. Beck and Nicolaides (1976) have allowed for discrete- and continuum-configuration correlation in their variational treatment of ions of the Li, N, and F sequences. Kastner (1976) has used the Coulomb approximation to calculate the strengths of forbidden transitions for ions of the B, F, Al, and Cl sequences. Mewe (1977) has presented tables of semi-empirical parameters for transitions along isoelectronic sequences of H through Al. Mühlethaler and Nussbaumer (1976) have used a scaled Thomas-Fermi potential with some configuration interaction for allowed and forbidden transitions of Be-like ions. Safronova (1976) has performed a charge-expansion perturbation calculation along the N sequence. Fischer (1976 and 1977) has applied multi-configuration Hartree-Fock theory to the calculation of oscillator strengths for the Al, Na, and Cu sequences. Armstrong, Fielder, and Lin (1976) have used multi-configuration Dirac-Hartree-Fock theory to predict f -values along the Li and Be sequences. Biemont (1977) calculated numerous transitions along the Li sequence by using a nonrelativistic Hartree-Fock approach. Schrijver (1977) applied a hydrogenic approximation with intermediate coupling to the calculation of inner-shell transitions of Li-like ions, while Fox and Dalgarno (1977) have calculated additional inner-shell transitions along the same sequence by means of the Z -expansion approach. Victor, Stewart, and Laughlin (1976) have used a semi-empirical model potential method with configuration interaction for low ions of the Mg and Ca sequences. Another group of papers contains data on highly ionized species of elements found in the solar corona. The HX (Hartree-Fock with statistical exchange) method of Cowan has been used by Bromage and Fawcett (1977) to calculate f -values of C-, N-, and O-like ions of Si, K, Ca, and Fe, and Bromage, Fawcett, and Cowan (1977) studied Fe X, XI, XVIII, and XIX with this approach. Flower (1977) has calculated allowed and forbidden transitions of Fe XI and XII, and Dankwort and Trefftz (1976) have applied Multi-configuration Hartree-Fock theory to Si X. Several papers are devoted to the calculation of neutral and/or weakly ionized species. Saraph (1976) has applied the frozen-cores approximation to a few transitions of Mg II and to numerous 1S - 1P transitions of neutral Mg. Biemont (1976) has applied a scaled Thomas-Fermi potential, and for some transitions a self-consistent field approach, to the calculation of f -values of doubly ionized species of Sc through Zn. Sinanoglu (1976) has reported results of his non-closed shell many-electron theory for transitions of many light atoms and ions. Bulatov (1976) has calculated A -values for microwave frequency transitions between fine-structure levels of the 2^3P term of He I.

The following theoretical papers are more recent and are therefore fully referenced. Lin, Johnson, and Dalgarno (7) have applied the relativistic random-phase approximation to several transitions of He-like ions. Shorer and Lin (8) utilized a Z-expansion approach to magnetic quadrupole transitions of the Be sequence, and Shorer has work in progress on the resonance lines of the Zn isoelectronic sequence, in which he considers the effects of the 3d subshell in particular. Lin, Laughlin, and Victor (9) have used model potential methods to calculate A-values of magnetic quadrupole transitions for Be- and Mg-like ions. Relativistic Hartree-Fock f-values were calculated by Kim and Cheng (10) for ions of the Na sequence. Fischer and Hansen (11) applied multi-configuration Hartree-Fock theory to the resonance transition of the Zn sequence, while Dankwort and Trefftz (12) applied the same method to the B sequence. Bromage, Cowan, and Fawcett (13) employed Cowan's HX method, including relativistic effects, for the calculation of f-values for Fe XII and XIII. Garstang, Robb, and Rountree (14) applied the close-coupling method with intermediate coupling to forbidden transitions of Fe VI, and Garstang reports further calculations in progress on Tc I. Nussbaumer and Storey (15) used intermediate coupling to compute A-values for allowed and forbidden transitions of C III. Nussbaumer has theoretical work in progress on a number of ions: N III, N IV, O V, F V, F VI, Ne VII, Ca XVII, Fe XXIII, Kr XXXIII, and Mo XXXIX. Dankwort (16) applied multi-configuration Hartree-Fock theory to the intercombination resonance line of Mg I. Pradhan and Saraph (17) calculated numerous oscillator strengths for O I using a configuration-interaction approach. At Brussels, van Rensbergen reports calculations in progress on C II, C III, and C IV, based on scaled Thomas-Fermi wave functions.

The following review of the recent experimental work is organized according to the techniques applied. Only the very recent papers not covered by the April 1978 NBS bibliography are referenced. Numerous direct measurements of transition probabilities have been performed by the traditional emission, absorption, and "hook" (anomalous dispersion) techniques. By means of emission measurements with wall-stabilized arcs, Wujec and Weniger (18) and Wujec and Musielok (1976) determined absolute oscillator strengths for prominent lines of Sn I and II, as well as for some Cl I lines. Kühne, Danzmann, and Kock (19) used a wall-stabilized arc to measure 56 Ti I lines. They combined their emission measurements with hook measurements. Czernichowski, Holys, and Roberts (1977) determined relative f-values for 27 ultraviolet Ne I lines with a wall-stabilized arc, and Ernst and Schulz-Gulde (20) performed a similar experiment for 23 Kr I lines. A special stabilized arc source was used by Lotrian, Cariou, and Johannin-Gilles (1976) to study 17 uv lines of Sn I, and Mosburg and Wilke (21) used a mercury discharge to determine the transition probabilities of 70 Hg I lines spread over a wide wavelength range. A number of measurements have been done by a simplified emission technique, the branching ratio method, in which the lines originating from a common excited atomic level are studied. The requirements on the light source are minimal; however, the relative transition probabilities obtained for these small sets of lines must be normalized by a lifetime measurement for the level in question (which has usually been obtained from beam-foil spectroscopy). In particular, Whaling, Scalo, and Testerman (1977), Lage and Whaling (1976), and Maier and Whaling (22) have applied such a combination of measurements to determine transition probabilities of Ti I, Pr II, and Nd II. Martinson, Curtis, Smith, and Biemont (23) used this technique on Mn II, Semenova and Smirnov (24) on Hg I, and Smirnov, Tsygir, and Yakovitskii (25) on neutral iodine. Using an advanced absorption technique, Blackwell and collaborators at Oxford are continuing their high precision measurements of relative oscillator strengths of neutral iron. More than 100 relative f-values for transitions arising from low excitation states have been measured with a precision as high as 1%, and a report is in preparation. Other recent absorption measurements are those of Bieniewski (1976) on Cr I, Bell and Lyzenga (1976) on Sc I (employing the atomic beam approach), and Hannaford and McDonald (26) on Cu I. Huber and Sandeman (27) used a combined approach of absorption and hook measurements to study 148 transitions of neutral chromium, with an overlap of the two approaches for some

lines of moderate strength. Hook measurements were performed by Parkinson, Reeves, and Tomkins, (1976) on Ca I, Sc I, Sr I, and Ba I, and by Smith and Kühne (28) on Ti I. Penkin and Komarovskii (1976) concentrated their hook measurements on neutral spectra of rare earth elements Nd, Sm, Eu, Gd, Dy, Tm, and Yb.

Many transition probabilities have been determined by measurements of the lifetimes of excited atomic levels. Due to the vigorous pursuit of beam-foil spectroscopy and due to the selective excitation capabilities of tunable lasers, this is currently a very active research area, with nearly 200 publications during the last three years, roughly half of them from beam-foil spectroscopy. Atomic lifetimes have been increasingly utilized to provide absolute scales for relative transition probability measurements. The high precision often obtained in lifetime measurements sometimes reaching the order of one percent, ties down absolute scales very accurately. The principal centres of lifetime measurements by beam-foil spectroscopy are the Universities of Aarhus, Alberta, Bochum, Kansas, Lund, Lyon, Quebec, Stockholm, Tennessee (Knoxville), Toledo, and Arizona (Tucson), and at the Argonne (Chicago), Darmstadt, and Berkeley laboratories. The new results are too numerous to be mentioned here individually. Instead, we note that many important new beam-foil results are covered in the Proceedings of the IVth and Vth International Beam-Foil Spectroscopy Conferences in Gatlinburg, Tennessee, 1975, and in Lyon, 1978, respectively. Furthermore, in the reviews by Curtis (5), Cocke (29), and Marrus (5) representative samples of recent results are discussed. In the usual beam-foil experiment, cascade effects are often encountered due to the non-selective excitation of atomic levels, which causes the measured lifetimes to be too long. A theoretical simulation study by Younger and Wiese (30) indicates that cascading effects are especially serious for $\Delta n = 0$ resonance transitions of heavy ions. Cascading is eliminated by the beam-laser approach. Two-stage excitation results from beam-gas cell and subsequent beam-laser interaction. The laser excitation is tuned to specific transitions. Schulze-Hagenest et al. (1977) determined the lifetime of the Li I $3d^2D$ level to within one percent with such a technique. Similarly, Arnesen et al. (31) determined some lifetimes of La II, again with very high precision. In conventional lifetime experiments, selective excitation with tunable lasers is also increasingly applied to eliminate the cascading effects associated with electron beam excitation. For example, Marek and Vogt (1977), Marek (32), Marek and Münster (33), and Hotop and Marek (34) used a pulsed dye laser for excitation and employed the delayed coincidence technique to analyze the decay curves from a number of Co I, Cs I, Sm I, and Dy I excited atomic states, work on Fe I is in progress. Teppner and Zimmermann (35) used an analogous technique to study some atomic levels of K I and Rb I, and Bulos et al. (36) applied it to some states of La I. A number of lifetimes were also measured directly by observing the exponential intensity decays from states selectively populated by one- or two-step dye laser excitation. Havey, Balling, and Wright (1976) studied lifetimes in Mg I, Al I, Ga I, Sr I, In I, Tl I, and Ba II; Gornik (37) measured some higher-lying levels in the Sr I spectrum, and Selter and Kunze (38) directly recorded the decay curves of some Al I and Ag I levels. Shaw, King, and Adams (39) determined lifetimes in Zn I and II with another version of the delayed coincidence technique, which also circumvents cascading effects. Still another refined version of the delayed coincidence method is the high frequency deflection technique, with which Brzozowski et al. (1976) determined a number of Fe I and II lifetimes, and Bromander et al. (40) measured lifetimes in C I, N I, and O I. An additional experimental method which has recently been applied is the Hanle effect (or zero-field level crossing) technique for measuring atomic lifetimes; for example the measurements by Kelly and Mathur (1976) on Sr I, by Bulos, Gupta, and Happer (1976) on K I, Rb I, and Cs I; by Rambow and Schearer (1976) on Mg II, Ca II, Zn II, Sr II, Cd II, Ba II, and Yb I and II (utilizing Penning ionization in a fast-flowing helium afterglow to generate the ions); by Becker, Bucka, and Schmidt (1977) on Cr I; by Klotz, Becker, and Goebel (41) on Co I; by Landais, Chantepie and Lanjepce (42) on Zn I; and by Andersen, Poulsen, and Ramanujam (1976) on Zn II, Cd II, and Hg II. The phase-shift lifetime measurement technique has been applied by Smith (43) to resonance transitions of F I, Si II, S I-III, and P II. Other specialized lifetime

measurements have been reported by Nowak, Borst, and Fricke (44) on O I, using a time-of-flight technique, and by Ramanujam (45), using a sputtering technique to study some levels of Fe I, Pb I, Zr I, and U I. Finally, it should be noted that Corliss and Tech (1976) have revised their extensive table of Fe I lifetimes on the basis of comparison with numerous recently measured values.

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WORKING GROUP 3: COLLISION CROSS-SECTIONS AND LINE BROADENING

A. *Line Broadening*

Stark broadening (1) and polarisation shift effect in high density plasmas (2) have been reviewed. Critical reviews and a tabulation of selected data of the Stark widths and shifts of lines of non hydrogenic atoms and ions have been published (32,33).

1. Broadening and shift of spectral lines of hydrogen and hydrogenic ions in plasmas.

Interest in Stark broadening of hydrogenic lines arising from dense, high temperature plasmas (2) - (11) is increasing for several reasons; one of them is the possibility of doing an experimental study of the far wings: this has enabled to evince predicted satellite structure (10). At high and low densities, the increase of experiments concerning the study of the center of the lines and the neighbouring wings have given convergent results (9), (11), (12), (13), (19) concerning the disagreement with theory. The importance of ion dynamics seems now well established: earlier experiments showing the dependence of the central dip of H β on the reduced mass have been confirmed (12), (13). Yet the various theoretical attempts of calculation have all failed (14) - (16), with the exception of the MMM (model microfield method), which enables a uniform semi-classical unified treatment of electrons and ion perturbers (17), (25): strong effects are found in the line centers of Ly α , H α and H β which agree with earlier experiments but not with the most recent ones (20). Another Stark broadening mechanism has been suggested for taking into account the mass effect (3): The importance of the interference term is still being debated (21), (22) and fine structure effects have been pointed out (12), (23).

The theory of the line wings of hydrogen lines has made great progress, with particular attention paid to the Ly α , Ly β , H β asymmetry (24) - (31). A detailed quantum calculation of the electronic broadening with a "dissection" of the various contribution has been made (24) - (26): in the far wings of Ly α electrons are predominant, short range and quantum effects are important; exchange is of drastic importance as well as quenching effects (27): this leads to the conclusion that the Holtmark limit is a fiction. In the near wings ions become important and an improved semi-classical approximation including dipole, quadrupole and quadratic (polarization) interaction gives a correct asymmetry for Ly α but not for Ly β when compared to the experiment (31). For H β the asymmetry calculated with the dipolar exact resonance theory (28) is in agreement with (11).

2. Broadening and shift of non hydrogenic atoms and ions in plasmas.

For isolated lines, experimental results of the two past years (34) - (46) (Ca II, Na I, He I, N I, C I, Si II, Al I, Al II, alkaline earth, Si III, IV, Ne II, F II, Cl III, Ar II, U V) have confirmed the success of the semi-empirical and semi-classical impact perturbation theories. The unitarized quantum distorted wave calculation (45) agrees with the semi-classical one (39). This confirms the fact that the high order terms included in the determination of the perturber's trajectory are of minor importance (47). The MMM has been applied to isolated lines (48), (53) and agrees with earlier impact theories.

For conclusion, theoretical and experimental widths and shifts agree within 20-30% with a few exceptions. The remaining discrepancies are attributed to the inaccuracy of the atomic structure of the radiating atom introduced in the calculations of the collisional profile. Interaction of configuration and fine structure effects have been pointed out (49), (50), but their estimation is not always sufficient to remove the discrepancy (39), (45), (49).

A number of works concerning the overlapping lines of He has been done (52)-(54). As for hydrogen lines, mass effects have been found in the dip between the forbidden and permitted components of λ 4471, (51), (52), suggesting the effect of ion dynamics: in fact the MMM (53) gives a correct dip when compared to the experiments. The satellite structure studied in (54) has indicated that the interpretation in terms of Baranger-Mozer plasma satellites has to be excluded: He₂ molecular transitions are proposed.

3. Collision broadening by neutral atoms.

Tables of damping constants of spectral lines broadened by H and He have been prepared for the needs of astrophysics; calculations are based on a Smirnov-Roueff potential (55).

Apart from these works the actual preoccupations seem to move away from direct astrophysical needs. The impact broadening of the central regions of atomic lines perturbed by various rare gases and the related relaxation and depolarization cross sections have been studied in great detail, both theoretically and experimentally (56) - (66). Sophisticated semi-classical calculations (56) - (58) have shown the importance of rotational and fine structure inelastic coupling and have explained the different behaviour of the lines of a multiplet (62). However the most striking fact is the drastic importance of the interatomic potential at low and medium distances on the results; a great number of efforts are now directed towards this problem: ab initio theoretical potentials (67) and more recently model potentials have been provided (68), (69). Short range effects being more important far from the line center, the relationship between the potential and the intensities in the wings has received great theoretical and experimental attention (66), (70) - (72). Attempts have been made to carry on an unified adiabatic theory for permitted lines (71), (72). The nearest neighbour static limit has been used to determine semi-empirical interatomic potentials from the wings of resonance lines (66), (70). Since the recent discovery (73) of strong laser excited molecular emission from alkali noble gases systems (excimeres) associated with the far wings of quadrupole and two-photons forbidden lines, a new research area is now quickly developing (74) - (79): the electric dipole moment of the formed quasi-molecule is very sensitive to the internuclear distance since it vanishes at infinite separations; its calculation has been made for several systems (75), (76). This ensemble of theoretical and experimental research in line broadening and molecular structure is providing new tests for theoretical adiabatic interatomic potentials originating from various excited states; eventual applications to laser physics increases the interest for this new branch.

4. Interaction matter-radiation: line redistribution and polarization studies (Zeeman and Hanle effect).

Several theoretical studies have recently been completed concerning the redistribution of radiation reemitted by atoms in the presence of collisions (80) - (83). Experimental studies have also been performed (61) and departures from the impact regime of the redistribution function have been measured (84), (85). In the impact approximation, the angular distribution of the scattered radiation has been studied in detail (80). The first theoretical attempts to study the non impact regime have been treated in (81)-(83), but numerical calculations have not yet been performed though results of (81) are in qualitative agreement with experiments.

The quantum theory of optical pumping (Hanle effect) has been applied for calculating the linear polarization of helium lines in solar prominences and the first results in terms of magnetic field diagnostic have been published (86), (87). An article reviewing the various spectroscopic regimes ranging from the low field Zeeman effect to the high field Landau regime has been published (88): the relationship with solid state physics and with astrophysics, in the application to the study of magnetic white dwarf stars has been discussed.

S. SAHAL-BRECHOT

B. Collisional Cross Sections

Data centres: Nagoya University Japan collects and publishes data for fusion, in Japanese. English translation will follow (K. Tayanagi). Bibliographies are distributed by the International Atomic Energy Agency Vienna (ordered according to process: photon, electron, heavy particle cross sections) (89), by JILA (heavy particle cross sections including charge exchange, but not reactions) (90), and by Oak Ridge National Laboratory. A bibliography on molecular data including cross sections is distributed as Berkeley Newsletters, see Report of Working Group 5, ref (1). New Centres in Daresbury, UK, and in Berkeley, Cal. (NRCC = National Resource for Computing in Chemistry) have been established who will supply programs for the computation of cross sections. State of the art information may be gained by the book on the invited papers of ICPEAC X, Paris 1977 (91) which contains 47 talks on all aspects. Many details are found in the corresponding books of abstracts (92) of contributed papers, and in (93). A survey over many aspects of atomic collision processes was given at a meeting in honour of Sir Harrie Massey's 70th birthday (94), e.g. Photodetachment (Lineberger), dissociative attachment (Chantry), highly excited atoms (Stebbins), reactions (Bernstein), charge transfer (Hasted), fast heavy particle collisions (Bransden), inner shell ionization (Burhop), atomic excitation (Heddle), theory of electron molecule collisions (Burke), thermodynamic effects in recombination (Bates), and atomic physics from atmospheric and astrophysical studies (Dalgarno). Reports on atomic collision research in Japan (95) come out annually. Sil (96) reports on atomic collision research in India as represented at the Centenary Symposium of Indian Association for the Cultivation of Science (1976). Direct application to astrophysics is given by Dalgarno and Black (97) and by van Regemorter et al. (98) on molecule formation and destruction in the interstellar medium where many processes are discussed. Diffuse clouds are treated in (99). The ratio of deuterated to normal molecules in different situations is discussed in (100). Unstructured charged particles (electrons, protons, α -particles) are dealt with in (101) where a simple formula for optically allowed transitions is given, and in (102) which calculates orbital angular momentum transitions in highly excited hydrogen.

1. Heavy Particle Collisions

Because of the size of the field this report is restricted to general information, review articles and some literature as it came to the authors notion. Many references had to be dropped. The reader will find them in the quoted literature.

Books: Two volumes on the dynamics of molecular collisions, edited by Miller (103), contain 13 articles, mainly on the theory of molecular collisions (Lester, Rabitz, Micha, Shin, Wolken, Siebrand, Porter and Raff, Kuntz, Hase, Child, Tully, Pechukas, Levine and Bernstein). In 1979 a book edited by Bernstein (104) on "Atom-Molecule Collision Theory: A Guide for the Experimentalist" will come out with articles by Child, Diestler, Kuntz, Levine and Kinsey, Light, H.F. Schaefer, Truhlar and Dixon, Truhlar and Muckerman, and Wyatt.

Reviews: Faubel and Toennies (105) deal with low energy vibrational-rotational excitation. A thorough review of the physics and mathematics employed by semi-

classical methods is given by Child (106) with many examples. Clark and Dickinson (107) use the Correspondence Principle to compare different approximations including the Strong Coupling Correspondence Principle approximation. De Pristo and Rabitz (108) stress especially the question of future lines of research as e.g. the "sensitivity" of "inversion" which means the reliability of extracting detailed molecular quantities from bulk properties. Truhlar and Wyatt (109) review H + H₂ energy surface and scattering. Many experiments have been done with laser excited atoms, especially Na(3²P^o), cf. Hertel and Stoll (110), who give a thorough theoretical introduction, and Hertel (111). Reactions and quenching of excited state atoms is described by King and Setser (112). Experiments of energy transfer of atomic excitation (Hg, alkali) to vibrations of the colliding molecule (H₂, O₂, N₂, etc.) are quoted by Lemont and Flynn (113). Highly excited "Rydberg" atoms ("free electron approximation", increase of lifetime by l-mixing) are dealt with by Edelstein and Gallagher (114) and by Takayanagi (115). Ion molecule reactions at thermal energies up to a few eV are reviewed by Ferguson (116) where many systems are quoted. A simple way of estimating charge exchange efficiencies at thermal energies on the basis of Landau-Zener approximation is mentioned by Dalgarno and Butler (117). Gayet (118) gives theory and rates for electron capture by protons at higher energies (25 - 200 keV). Different approximations for high (~10 keV) and low (~0.1 keV) energy are described and results compared with measurements by Basu et al. (119). Bobashev (120) considers quasi-molecular interference effects in ion-atom collisions and their effect on the polarization of emitted light. The excitation of inner shells in slow atomic collisions ($v < v_{\text{electron}}$, 1 - 100 keV) is discussed by Briggs (121). Reactive rearrangement collisions are mainly treated by statistical methods and chemical models, cf. Bernstein (94). Goldanski (122) shows that at very low temperature ($\lesssim 20$ K) activation energies of molecular reactions may go down, polymerisation may happen. Klein (123) describes isotope effects (mainly H-D) in chemical reaction rates quoting ratios of reaction or quenching rates. Bauer (124) gives a theory of chemical reactions including multiple scattering. Drift tube experiments of ion-molecule reactions at thermal energies (0.01 - 1 eV) are reviewed by Biondi (125).

In many papers the importance of the energy hypersurface describing the collision system has been stressed. Refined programs for ab initio calculations exist (126), (127). Electron cloud models together with asymptotic terms for large distances are suggested in (128), (129). A "Diatomics in molecules" model is used for H₂⁺(D₂⁺) + H₂(D₂) (130). Adjusted to measurements is the model (131). With sufficient theoretical background potentials may be extracted from scattering experiments for the spherically symmetric part of H₂-H₂, H-rare gas, H₂-rare gas cf. (132), (133). The stability of negative ions of polar molecules is discussed in (134).

Full close coupling quantum mechanical calculations for rotational excitation have been done for H₂-H₂ (135). For heavier systems the restriction to one input channel may allow an increase in the number of channels (136). Otherwise the number of coupled channels has to be reduced by some approximation. A few examples are given which guide to further literature. The "Coupled States" method (diagonalizing the body fixed centrifugal term) has been used to study He - HCN, Ar - N₂, Ar - HCl, H⁺- H₂ (137,138), He - HCl (139). A similar method ("decoupled l-dominant" method), suited for strong long range forces, has been applied to Ar - N₂, Li⁺- H₂ (140). A generalization is given in (141). A method suggested by Tang is applied to Ar - N₂, H⁺- H₂ (142). Sudden approximations are used to study the influence of the anisotropic part of the potential (143,144). Further systems (e.g. H₂-CS, H₂-OCS, He-HCN, He - N₂H⁺) are studied (145,146). Higher energies (a few eV), including vibrational excitation are considered for Li⁺-H₂ (147), for He-O₂, He-H₂ (148), for H₂-H₂ (149), and for H₂-He (150). Classical path calculations have been done for Li⁺- CO (126), for He - NH₃ (151), and for CO₂- He, Ar (152). K - NH₃ has been observed (153) and vibrational excitation of many atmospheric gases by H⁺, impacting on CO, CO₂ (154) and by Li⁺ on CO₂, N₂O (155), on H₂, D₂, N₂, O₂, CO, CO₂ (156). NO⁺ vibration is

efficiently quenched by N_2 (157,158), CO by aromatic hydrocarbons (159) and by O (160). Special attention has been paid to the system $H^+ - H_2$ experimentally (161) and theoretically (162). The cooling of hot interstellar gas by H_2 is discussed in (163). "Surprisal" analysis is used to generalize calculated results for special rotational transitions to others (164). Fine structure transitions are important for the cooling of interstellar clouds and for lasers. The following systems have been calculated: $H-C^+$, H_2-C^+ (165), $H-C$, $H-O$ (166), $F-H_2$ (167). $I - H_2O$ (168) was measured. For classical path calculations involving a change of the energy surface complex trajectories through the complex crossing point of the surfaces might be useful (169). Fine structure transitions in excited alkalis are measured for Na 4^2D - rare gas (170). Deexcitation of alkali 2^2P states by N_2 , H_2 , O_2 is calculated in (171) and measured in (172). Elastic scattering of metastable He 2^1S on rare gases has been measured (173), also ionization of rare gases by He 2^1S , 2^3S (174). Ionization of Ar by He 2^2P is calculated in (175). The deexcitation of metastable highly charged hydrogenic ions (Mg XII, P XV, 2^2S) has been calculated (176). In collisions with highly excited "Rydberg" atoms the outermost electron may be treated as free (177). Ionizing collisions between Rydberg atoms are calculated in (178), and between a Rydberg atom and a polar molecule in (179). Electronic deexcitation of molecular $N_2 A^3\Sigma_u^+$ by N_2 , Ar, H_2 is reported in (180). A formalism to treat such cases theoretically is given in (181). Ionization of H_2 molecules by H_2 , N_2 at 0.2 to 5 keV was measured (182).

Many measurements and calculations refer to ion-atom, ion-molecule collisions. Rate constants between an ion and a polar molecule may be estimated by the "average dipole orientation" theory (ADO) which is improved in (183) for proton transfer reactions. For very low energies (< 1 eV) charge exchange cross sections may have a minimum, e.g. for Ne^+ , $Ar^+ - Ar$, Kr (184), cf. also $H^+ - D$ at 1 to 30 meV (185). For higher energies (< 200 eV) charge exchange cross sections for H^+ and rare gas ions in neutral rare gases are given in (186). A prescription how to correlate diabatic states of the electron exchanging system between small and large distances of the particles is given in (187). Charge exchange measurements with molecules are described for $Ar^+ - O_2$ at low energies (~ 1 eV) (188), and for C^+ , N^+ , $O^+ - N_2$ at 700 eV (189). An improvement on molecular theory for ion atom collisions is given in (190). Of great interest are charge exchange collisions with highly ionized species as calculated for $O^{+8} - H$ at 0.025 to 200 keV (191), and for H-like - H at 4 to 200 keV (192). A theoretical discussion is given in (193) for e.g. HeH^{++} up to 50 keV. At high energies the electron may also be captured into a free state (194). Electron detachment from H^- in collisions with H, He have been calculated for energies of 10 keV to 10 MeV (195). Ionization of hydrogen by protons is calculated in (196) at 25 keV and 200 keV. Ionization of He by Li^+ at 2 to 5 keV was measured (197). Charge exchange may be accomplished by a radiative transition. Calculations have been done for $H - C^{++}$, C^{+++} , N^{++} at energies up to 10 eV (198). A semiclassical theory of radiative excitation transfer is given in (199). Radiative association of $C^+ - H$ has been calculated for temperatures of 20 to 1000 K in (200). Three dimensional calculations of the $H - H_2$ reactive system are reported (142,201). The following reactions have been measured: $HCO - NO$, O_2 , thermal (202), $O^+ - N_2$, O_2 , 300 to 900 K (203), $CN - NO$ (also in excited vibrational states) (204), O_2^+ , NO^+ , $O^+ - CO_2$, N_2 , CO, H_2 , Ar, NO, O_2 , thermal (205), $H_2CO - Ar^*(4^3P) \rightarrow CH^*A^2\Delta + \dots$, thermal (206), $N-NO$, 200 to 400 K (207), $O-I_2$, CS_2 , OCS, 50 to 300 meV (208). A statistical theory of ion-molecule reactions is given in (209). The spontaneous dissociation of H_2CO from excited levels is calculated in (211) and of H_2CO^+ in (210). For some molecules which can't be directly observed by radio astronomy protonated ions may be important (212). The proton affinity has been measured for CS in (213).

E. TREFFTZ

2. Electron collisions with, and photoionization of, molecules.

New results of general interest are being produced by the technique of laser

photoelectron spectrometry (214) - (217). Experimental low-energy electron scattering results have been reported, including rotational and vibrational excitation, and for some strongly polar molecules (218) - (221). A small number of low-energy cross-section calculations have been reported, including LiF, H₂, F₂ and CO₂ (222) - (225). Further results should soon be available from R-matrix calculations (226). There are calculations of dissociative excitation for H₂ (227) and H₂O (228) - (230). Photoionization calculations have been reported for H₂ and N₂ (231) - (234).

3. Electron collisions with, and photoionization of, atoms and ions.

A bibliography for electron - positive ion collisions (1940 to 1977) is found in (235). Useful reviews include: physical processes in planetary nebulae (236); atomic processes in hot plasmas (237); empirical formulae for excitation and ionization (238), (239); dielectronic recombination (240), dielectronic satellite lines (241); experimental ionization results (242), (243); ionization experiments and theory near threshold (244), (245); excitation of C and O ions (246).

The potentials to be used in collision calculations have been considered (247) - (251). Resonance contributions to excitation cross-sections have been considered (252). The Bethe approximation has been reviewed and generalised (253), (254). The importance of inner - shell contributions to ionization cross-sections has been stressed (244), (255), (256). A method of analytic evaluation of Coulomb Born integrals avoiding partial wave analysis has been given (257), (258). The accuracy of close-coupling and distorted wave calculations for special test cases has been assessed (259) - (263). Details of one of the standard close-coupling programmes have been published (264). The variable phase method of solving the close-coupling equations has been discussed (265). Experimental measurements of excitation cross-sections include: the resonance lines of K, Rb, Cs (together with polarization measurements and data on H, Li and Na) (266); 2s - 2p in C³⁺ (267); 2³P emission cross-section for Li⁺ (268); resonance lines of Sr, Ba and of Sr⁺, Ba⁺ (by electron impact with the neutral species) (269), (270). Close-coupling calculations have been reported for excitation of: C⁺ (2P_{1/2} - 2P_{3/2}) (271); C²⁺ (272); C³⁺ (273), (274); N⁴⁺ (275); O⁺ (forbidden) (276); O⁴⁺ (272); Ne⁷⁺ (277); Ar¹⁵⁺ (274); K (278); S⁺ (forbidden) (276). Distorted wave calculations have been carried out for excitation of atoms and ions too numerous to detail, see (279) - (289) and references therein. Similarly, for Coulomb-Born calculations, see (290) - (295).

Experimental ionization cross-sections have been measured for C³⁺ and N⁴⁺ (296); some results have also been inferred from plasma observations (297) - (299). Ionization cross-sections for highly charged ions have been calculated in the Coulomb Born approximation (300), and autoionization rates (and fluorescence yields) have been calculated for Li-like ions (301). Experimental measurements of dielectronic recombination in Fe⁸⁺ to Fe¹⁰⁺ have been reported (302). Calculations including the effect of autoionization with excitation have been made (303), (304). Results for He-like ions have been given (305), (306). The effects of microfields and collisions have been considered (307), (308). Several calculations of ionization balance and level populations in plasmas contain useful results on collision cross-sections and other atomic data, see (309) - (318). Photoionization measurements for O, Al, Fe and Ba (319) - (322), and calculated results for H⁻, C, N, O, F⁻, Ne (323) - (328) and a range of positive ions (329), (330) have been reported. Semi-empirical results for He are in (239).

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A. BURGESS

Chairman of the Working Group

WORKING GROUP 4: STRUCTURE OF ATOMIC SPECTRA

A. *Compilation and Bibliographies on Energy Levels, Wavelengths, and Line Classifications*

The ongoing program of the Atomic Energy Levels Data Center (National Bureau of Standards) to produce new compilations of critically evaluated energy level data is at present focused on the first thirty elements. The most recently completed compilations in this series give energy levels for all the spectra of Mn (Mn I-XXV) (1), Cr (Cr I-XXIV) (2), V (V I-XXIII) (3), Ti (Ti I-XXII) (4), Ca (Ca I-XX) (5), and Al (Al I-XVIII) (6), and work is underway on the spectra of K and Mg. C.E. Moore's "Selected Tables of Atomic Spectra" now include O I (7), O VI, O VII, and O VIII (8), work on the tables for the remaining oxygen spectra is in progress. A finding list for lines of the multiplets in Sections 1-7 of Moore's NSRDS-NBS 3 series has been compiled by Adelman et al. (9). A recent publication of the AEL Data Center, "Atomic Energy Levels - The Rare-Earth Elements" (10), gives energy-level data for 66 spectra of the 15 elements La through Lu ($Z=57-71$), including a number of astronomically important spectra. A review of rare-earth spectral data by Blaise et al. (11) gives partial tables of energy levels and wavelengths and includes data on hyperfine-structure and isotope shifts. The first version of a much needed new compilation of "Line Spectra of the Elements" has recently been published (12). These tables contain some 42,000 lines, including the stronger lines of the first and second spectra of 98 elements and lines of the third, fourth, and fifth spectra for about half the elements from the vacuum ultraviolet to the far infrared. Outred (13) has compiled 8885 selected lines of 57 elements in the infrared region 1-4 μm , with energy-level classifications being given where available. Energy-level and Grotrian diagrams for the atoms and positive ions of the elements H through P ($Z=1-15$) have been prepared by Bashkin and Stoner (14), and further publications for the heavier elements are planned. The AEL Data Center (NBS) expects to publish in 1979 a "Bibliography on Atomic Energy Levels and Spectra" for the period July 1975 through December 1978 (15). Edlén's 1976 review of term analysis of atomic spectra has references for spectra of the elements He through Ni (16), and Adelman et al. (17) have compiled an astronomically oriented bibliography on atomic autoionization. A bibliography on experimental isotope shifts in atomic spectra by Heilig (18) gives 666 references.

B. *Laboratory Research*

Reports on the research programs of a number of laboratories have been received. The present report is highly selective and incomplete regarding references to research on particular spectra, since the forthcoming bibliography (15) fully covers such references and will be widely available to astronomers.

I. Selected References, $Z \leq 28$

The references in Table 1 (in parentheses following the spectra) are a partial list of recent results for the elements through Ni. Several additional references for extensive isoelectronic-sequence results and a few references for spectra of heavier elements are given below.

II. Isoelectronic Sequences

Erickson (19) has calculated accurate energy levels for the one-electron species

TABLE 1

Selected references on energy levels and line classifications, $Z < 28$

B I (33)	Ca V-VIII (46)	Mn XIX (69)
	Ca X (49-51)	Mn XXII (58)
F I (34)	Ca XIV (52)	Mn XXIII (64)
	Ca XV (44,52)	
Na IV (35)	Ca XVI, XVII (53)	Fe I (70,71)
		Fe II (72-75)
Mg XI (36)	Sc I (54)	Fe IV (76)
	Sc VI-IX (46)	Fe V (77)
Al V (37)	Sc XI (50)	Fe IX (78,79)
Al XII (36)	Sc XVI (44)	Fe X (46,78,80,81)
		Fe XI (46,81)
Si V (38,39)	Ti III (55)	Fe XVI (82)
Si VI (40)	Ti V (56)	Fe XVII (83)
	Ti VII-X (46)	Fe XVIII (83,84)
P III (41)	Ti XII (57,50)	Fe XIX (82-86)
P IV (42)	Ti XVII (44)	Fe XX (69,83,86-88)
P VI (43)	Ti XIX (58)	Fe XXI (44,83,86,87)
P X (44)		Fe XXII (61,87)
P XIV (36)	V II (59)	Fe XXIII (58,61)
	V VI (60)	Fe XXIV (64)
	V VII-XI (46)	
S I (45)	V XIII (50)	Co VI (89)
S IV (46)	V XVIII (44)	Co X (79)
S VII (47)	V XX (58,61)	Co XX, XXI (69)
S XI (44)		Co XXIV (58)
S XIV (48)		
S XV (36)	Cr III (62)	
	Cr VII (63)	Ni IV (90)
Cl XII (44)	Cr VIII-XI (46)	Ni V (91,92)
Cl XVI (36)	Cr XIV (50)	Ni VII (93)
	Cr XXI (58)	Ni X (79)
Ar XIII (44)	Cr XXII (64)	Ni XI (78,79)
		Ni XII (78)
K IV-VII (46)	Mn III (65)	Ni XVIII (82)
K IX (49,50)	Mn V (66,67)	Ni XXI (82,86)
K XIV (44)	Mn VI (68)	Ni XXV (58)
	Mn IX-XI (46)	Ni XXVI (64)
	Mn XV (50)	

of all atoms (H I sequence, $Z = 1-105$), and Vainshtein and Safronova (20,21) tabulate calculated wavelengths and transition probabilities for the He I and Li I sequences up to $Z=34$. Experimental wavelengths and energy-level classifications have been given by Boiko et al. (22) for about 1000 lines belonging to ion spectra of the H I ($Z=12-16$), He I (11-26), Li I (19-26), Be I (22-34), and Ne I (26-42) sequences. A semi-empirical treatment of the Li I sequence by Edlén (23) gives energy-level and wavelength data for line identifications ($Z=3-28$). Edlén has also obtained expressions for the Na I sequence predicting the 3s-3p and 3s-3d transitions and the ionization energies ($Z=16-42$) (24). Edlén's predictions of the ground-term 2P intervals for the F I and B I sequences ($Z=24-42$) (25) can be used for the identification of the corresponding forbidden lines.

III. Brief Report on Laboratory Programs

The following notes on current research of astrophysical interest are mostly excerpted from information supplied by the persons whose names appear in parentheses. At the University of Lund, work is almost complete on the spectra O II, P I, II,

S II, Sc II, Ti II, and Ga II, and work in progress includes B II, F II, III, S IV-VI, Cl IV-VII, Sc V-Fe X (sequence), Ti I, Cr IV, V, Fe II, III, VII, VIII, and Ni I (U. Litzén). Spectra under investigation at the Lund Institute of Technology include O III, Ne III, Ar III, IV, and K II (L. Minnhagen). Extensive research on highly ionized atoms from laser-produced plasmas is continuing at both the Lebedev Physical Institute and the Institute for Spectroscopy, U.S.S.R. Academy of Sciences, and predicted wavelengths of forbidden lines (1800-10,000 Å) are being obtained (S.L. Mandelstam, M.A. Mazing). Laboratory spectroscopy in the Astrophysical Research Division, Culham, is concentrated on highly ionized iron-group atoms, especially V, Fe, Co, and Ni (B.C. Fawcett). Spectra of ions of Al and Si are under investigation at the Paris-Meudon Observatory, with work on Al VI nearing completion, and a compilation of forbidden transitions of astrophysical interest is in progress (M.-C. Artru, M. Eidelsberg). Autoionization and photoionization spectra are among the areas emphasized at the Harvard-Smithsonian Center for Astrophysics, with a new ion-beam facility being used for investigations of multiply charged ions (J.L. Kohl, W.H. Parkinson). Work on Co II and Ni III is almost complete at the Institute of Optics, Madrid, and V II and Cr II, III are among the other spectra now being analyzed (L. Iglesias). Papers on Co IV, V, VI, Cu VI, and Er I, II have been submitted or are being prepared at the Zeeman Laboratory, Amsterdam, and spectra under investigation include Mn IV, Ni VI, Cu VII, and Tb I, II, III (E. Meinders, T.A.M. van Kleef). A number of complex spectra are being analyzed at the Aimé-Cotton Laboratory, Orsay, including Pr I, II, and Yb I; an extension of the Lu I analysis has been published (26) (J. Blaise, J.-F. Wyart). Accurate ionization potentials for most of the neutral rare-earth atoms have recently been determined at the Lawrence Livermore Laboratory, University of California, by use of laser techniques (27), and regularities across the f-shell rows yielded predicted energies in higher ions (28). Work in the Theoretical Chemistry Dept., Oxford, is centered on accurate relativistic calculations of low-energy states of heavy atoms (29); a number of related computer programs have been made available (30) (I.P. Grant). From the Dept. of Theoretical Physics, Oxford: A recent review of the atomic physics of astrophysical plasmas has a useful section on energy levels and line identifications (31) (C. Jordan). Energies in H⁻ and He I (32) have been calculated at the Centre for Research in Experimental Space Science, York University (H.O. Pritchard).

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WORKING GROUP 5: MOLECULAR SPECTRA

A. *Compendia, Bibliographies and Atlases*

Molecular spectroscopic activity, and its literature, has continued to proliferate strongly during the reporting period. There has been much work over the entire wavelength range: microwave - extreme ultraviolet. The impact of the methods of laser spectroscopy on the field, and developments in molecular lasers have continued to provide a great stimulus to molecular spectroscopic research. There has also been increasing recognition of the need for fundamental spectroscopic data of all kinds in astrophysical, atmospheric and environmental research applications. The scope of contemporary interests is displayed in the programme books for the symposia on Molecular Spectroscopy held annually at the Ohio State University. For the past three years the literature of the molecular spectroscopy has been so prolific that it is impossible to make a definitive review even of the astrophysically important contributions beyond brief citations. Important trends are indicated below. Literature citations have been principally compiled from the reports received from individual workers in Centres of Research on molecular spectra.

The bi-monthly Berkeley Newsletter (1) compiled by Phillips and Davis from more than 30 journals continues to be distributed to about 500 workers. It gives most valuable access to the literature of the spectra of small molecules. Recent copies reference 200-300 papers, books, etc. The wide need for reliable compilations, for a critical assessment of molecular data has been increasingly emphasized during the past few years. Herzberg and Huber (2) report the publication of a long anticipated volume "Constants of Diatomic Molecules" which makes a critical assessment of the literature and significantly updates the tables of Herzberg's "Spectra of Diatomic Molecules", published in 1950. Hsu and Smith (3) have made an important review of spectral data of visible and ultraviolet diatomic molecular spectra of astrophysical interest. Nicholls (4) has reviewed transition probability data for astrophysical molecules. Lofthus and Krupenie (5) have compiled data on the spectrum of N_2 . The identification of molecular spectra has continued to remain an important problem. Pearse and Gaydon (6) have published in 1976 the fourth edition of "The Identification of Molecular Spectra". Kopp, Jansson and Rydh (7) have published a table of band features of diatomic molecules which is a supplement to the 1974 edition, cf. the 1975 report of this Committee. Spectral atlases continue to be produced. Hsu, Monts and Zare (8) have published a spectral atlas of NO_2 . Park (9) has produced a spectral atlas of infrared absorption lines and Nordstrom, Shaw, Skinner, Calvert, Chan and Uselman (10) have published an atlas of air absorption in the infrared between 700 and 2300 cm^{-1} . Roney et al (11) and Benedict (12) have recently commented on the data in the Air Force Geophysical Laboratory atmospheric absorption line parameter compilation. Two important books on Molecular Spectroscopy have recently appeared: "Diatomic Molecules, Results of ab initio Calculations" by Mulliken and Ermler (13) and "Molecular Symmetry and Spectroscopy" by Bunker (14).

B. *Molecular Data*

During the past three years there has been a continued emphasis on diatomic molecules of astrophysical, atmospheric and laser importance. Herzberg and Huber's "Constants of Diatomic Molecules (2) is an invaluable contribution to this area. Whiting et al. (15) have made recommendations for clear definitions of transition moments and intensity factors in the spectra of diatomic molecules. The diagnostic applications of molecular spectroscopy to stellar atmospheres calls for a continuing critical assessment of the thermochemical data available for stellar molecules. The need for better data in this field has been strongly emphasized by Sauval and Tatum. Similarly high quality data on excitation cross-section data for diatomic molecules are needed. Ames and Huebner (16) report studies on emission cross-sections for rotational transitions. There has been continued interest on potential energy curves for diatomic molecules. Kuriyan and Pritchard have made numerical studies

on potentials H_2 (17,18). Schadee reports studies on the Zeeman effect in electronic transitions of diatomic molecules (19). Hefferlin (20) has continued studies on a periodic table for diatomic molecules. There has been a continuing research effort on *ab initio* quantal calculations on the properties of many diatomic molecules. Important developments in this field are being made at the NASA Ames Research Center, at the Argonne National Laboratory and the IBM Research Center San Jose.

I. Electronic Band Analyses and Constants of Diatomic Molecules

Coxon and Sastri are making a comprehensive attempt consistently to fit all of the available scientific data on OH by one model. Tatum continues analyses on bands of TcO. Dressler reports analyses of H_2 (21), N_2 (22) and N_2^+ (23) states. Barrow reports studies of CuF (24), FeF (25), CeO, SiS and FeO. Kotlar has made an extensive analyses of the CN Red Band System using Berkeley data (26). Linton reports analyses of TiO systems (27,28), SiO systems (29,30) and on one system of YO (31). Jordan (32) reports collaborative studies of CO fluorescence and lines of H_2 in the extreme UV solar spectrum (33). Lew (34) has made analyses of singlet systems and measurement of dissociation energy of NH and ND. Brown reports studies on the He_2 (35) and Ag_2 (36) molecules. Benesch reports high resolution studies on N_2^+ bands (37) and infrared N_2 bands (38,39,40). Lindgren reports analyses of MgH and MgD spectra (41) and identification of FeH in the spectra of M dwarfs and S stars (42). Ramsay reports analyses of the vibration-rotation spectrum of HD (43) and a r-analysis of the ClO system (44). Shaw (45,46) reports methods of band analyses using computer graphics display terminals. Leach reports analyses of CS bands (47).

II. Transition Probabilities, Lifetimes, Intensities

Two sets of suggestions for uniformity of definitions concerning transition probability data for diatomic molecules have been made recently. Schadee (48) has proposed uniform definitions of band strengths of diatomic molecules and Whiting et al. (15) have proposed uniform definitions for Hönl-London factors and electronic transition moments for diatomic molecules. Numerous high quality measurements of lifetimes have been made for the upper states of many transitions of astrophysical interest. These include extensive work by Erman and colleagues in Stockholm using the high frequency deflection technique (49) which allows lifetime measurements of individual rotational levels. Erman reports work on CH^+ (50), other hydride ions (51), other hydrides (52,53,54), I_2 (55), C_2 (56), N_2^+ (57) and NO (58). Instrumental and review aspects have been discussed (59,60,61). Predissociation and perturbations studies have been made (62,63,64,65). Thrush et al have made lifetime measurements on excited BO and BO_2 (66). Llewellyn (67) reports lifetimes measurements on OH and excitation kinetic of the IR atmospheric O_2 bands (68) and quenching of OH (69). Leach et al (70) report lifetime measurements on C_2 . Linton (71) reports lifetime measurements on TiO. Davis also reports lifetime measurements on the TiO α and β systems (72,73). Sulzman has made shock tube measurements of oscillator strengths of TiO α and γ bands (74), and of vibration-rotation bands of AlO (75). He reports high temperature absorption coefficient measurements on methane (76) and non-LTE spectral absorption coefficients for vibration-rotation bands of diatomic molecules (77) and on other electronic bands of diatomic molecules (78). Benesch reports absolute oscillator strength measurements on bands of N_2 (79). There have also been a number of photoelectron spectroscopy measurements of cross-sections for various astrophysical band systems. Marr (80,81) reports such measurements for N_2 using synchrotron radiation, Samson et al have made photoelectron studies of H_2 (82), N_2 (83), O_2 (84), O_2^+ , N_2^+ , CO^+ (85), CO_2 (86), CO (87), O_2^+ (88). Gattinger reports synthetic spectral studies of O_2^+ (89), O_2 (90) and N_2 (91) in the spectrum of the aurora. Shaw reports intensities and widths of H_2O (92) and N_2O , CO_2 , CO and H_2O (93). Carver (94) reports oscillator strengths and line-widths for O_2 Schumann-Runge bands. Arnold et al (95) have made shock tube measurements of SiO transition moments. Smith et al. report refractive index measurements on H_2 , He, O_2 , CO and Kr

(96). Johnson reports transition probability studies of N_2 (97). Stoicheff reports laser excited fluorescence studies on CO and lifetime measurements of perturbed levels (98). Ab initio theoretical studies on SiO (99), C_2 Swan Bands (100) and HOCl (101) are reported by Arnold. Rumble (102) has made studies on bounds on the oscillator strength of H_2 . Dalgarno reports calculations of oscillator strengths (103) for Li_2 and Na_2 (104) for alkali hydrides (105), of potential curves for Li_2 (106), for potential curves for two electron systems (107), and vibration-rotation transition probabilities for H_2 (108).

III. Polyatomic Molecules

A wide variety of polyatomic studies in the radio frequency, infrared, visible, and ultraviolet regions of the spectrum have been reported. Ramsay reports observations on NH_2 (109), glyoxal (110), diacetylene (111), formaldehyde (112), and NH_2 (113). Oka describes detection of cyanohexatriyne (114), and observations on cyanodiacetylene (115,116). He reports work on forbidden infrared transitions using two photon laser resonance spectroscopy (117). Observations were made on NH_3 (118, 119,120) and HCO (121). Lees reports microwave double resonance studies on OCS (122,123, 124), on methanol (125,126), on methane (127), and on silane (128). Gerry reports microwave studies on isocyanic acid (129), silane (130), cyanacetylene (131), cyanogen isocyanate (132), propyolic acid (133), and HNCS (134). Lutz reports on high resolution infrared studies on methane with application to atmospheres of planets (135,136,137,138). Leach reports studies on the optical spectra of molecular ions (139), CO_2^+ (140), and CS_2^+ (141). McDowell reports continued work on the photoelectron spectroscopy of small molecules (142,143) such as the diazenes and the imines which are of potential astrophysical interest, although they have not yet been identified as interstellar molecules due in part to lack of knowledge of their microwave spectra.

RESEARCH IN PROGRESS

A. *From the National Research Council of Canada* (reported by G. Herzberg and A.E. Douglas)

Spectroscopic studies of molecules of astronomical interest continue to be the major interest of the laboratory.

Absorption and emission spectra of HD in the vacuum uv have been investigated (156), the emission spectrum of H_2 is being remeasured with greater accuracy. Experimental studies of the infrared vibrational spectrum of HD (161) and the rotational quadrupole spectrum of H_2 (182) have been completed together with theoretical studies of the HD spectrum (158) (180). The vacuum ultraviolet absorption and emission spectra of the diatomic molecules F_2 (159) and Cl_2 (151) have been investigated and the near ultraviolet spectrum of ClO has been re-investigated in more detail (157). The absorption spectrum of BeH has been described (154) and some of the perturbations in the $B^2\Sigma$ state of CN have been explained (150). Two review papers on the spectrum of NO have been published (164) (166). A number of papers have been published on the electronic spectra of the diatomic molecular ions HF^+ (145), NO^+ (146), O_2^+ and N_2^+ (169) and on the calculated infrared spectrum of HeH^+ (170). A detailed analysis of the electronic spectrum of H_2O^+ (163) and a measurement of the lifetime of the excited state (149) have been published. An extensive study of the electronic spectrum of $HeNe^+$ has just been completed (184). Further investigations of the electronic spectra of the polyatomic molecules NCO (144), NH_2 (147) (148) (162), NO_2 (174), HNO (165) and C_4H_2 (171) have been reported. Considerable effort has been devoted to the study of the infrared spectra of molecules by the laser-Stark and laser-Zeeman methods since this work can give accurate frequencies of infrared lines which are of interest for infrared astronomy. Studies have been reported on the spectra of H_2CO (173) (178), HDCO (168) (183), NO (153), HCO (177) (179), HNO (167), HO_2 (181) and work is in progress on H_2CNH . In addition double resonance and two-photon experiments have given similar information on the infrared spectra of NH_3 (160) (175), NO (176) and SiH_4 (152) (155). A study

of the absorption spectrum of CH_3D in the 6000-12000 \AA range has been published (172).

B. *From the National Bureau of Standards*
(Reported by Frank J. Lovas)

a. Data Assessment, Reviews, Atlases

The molecular spectra data center at NBS has a continuing program to develop critical reviews, some of which specifically deal with the spectra of interstellar molecules. Some of these are carried out at NBS and others by spectroscopists at other institutions. Recent critical reviews published in the *J. Phys. Chem. Ref. Data* series "Microwave Spectra of Molecules of Astrophysical Interest" cover the microwave spectra of CH_3CHO (185), HNCO (186), SiS (187), OH (188), HCCCN (189), and $\text{CH}_2=\text{CHCN}$ (190). The major feature of these reviews is to provide the fundamental data needed for identifying and interpreting interstellar observations. Predicted spectral lines are given in addition to the observed frequencies in order to provide complete frequency coverage. Work is in progress on CH_3CCH , and CH_3CN (191), HCOOH (192), HCOOCH_3 (193), CH_3OCH_3 (194). A new compilation entitled "Recommended rest frequencies for observed interstellar molecular lines", is close to completion (195). An extensive critical review of the microwave spectra of 54 triatomic molecules has been completed and will appear as Part II of the "Microwave Spectral Tables" (196). The review contains spectral data on the interstellar molecules H_2O , H_2S , OCS , HCN , HNC , HNO , HCO , HCO^+ , HN^+ and SO_2 . A new NBS compilation on high resolution infrared has been started by W. Lafferty and A. Maki. The first review will treat selected diatomics: CO , CS , ClO and the hydrogen halides. An extensive compilation of the NO spectrum is also in progress by Guelachvili. In the area of electronic spectra an atlas of the absorption spectrum of NO (197), and a definitive review of the spectrum of N_2 (198), have been published recently.

b. Molecular Data

1) Microwave region

Isotopic forms and the molecular structure of CH_2NH has been studied (199). Measurements of the millimeter spectrum of $\text{C}_2\text{H}_5\text{CN}$ assisted its identification in interstellar sources (200). The laboratory microwave spectrum of NH_2CN has been reported (201). New measurements of the microwave spectrum of $^{14}\text{N}^{32}\text{S}$ and $^{14}\text{N}^{34}\text{S}$ have been completed (202).

2) Far infrared region

Laser magnetic measurements of the rotational spectrum of CH have been carried out at NBS-Boulder (203). Work is now in progress on CH_2 by K. Evenson and co-workers.

3) Infrared region

The 2-0 vibration-rotation bands of $^{12}\text{C}^{32}\text{S}$ and $^{12}\text{C}^{34}\text{S}$ near 2530 cm^{-1} have been reported (204) and a high resolution study of the 1-0 bands with a diode laser spectrometer has just been completed (205). A high resolution study of HNC in equilibrium with HCN has been completed by Maki and Sams (206). Jacox has published a matrix isolation study of the infrared spectrum and structure of the CH_3 free radical (207).

C. *From the University of California, Berkeley*
(Reported by J.G. Phillips and S.P. Davis)

1. Molecular Analyses

High resolution Fourier transform spectroscopy has been used to study the emission spectrum of TiO between 4000 \AA and 3 μm . The analysis of the ψ -system has

been completed. About 3000 lines from 25 bands have been identified. Molecular constants have been calculated. Band intensities agree well with predicted Franck-Condon factors and known isotope abundances. 19 new bands of the (${}^1\Pi-1\Sigma$) system of ZrO have been identified from 5849 Å to 8179 Å. The system should be present in S-type stars. Our observed isotope shift for the $v = 2$ sequence agrees with calculations. 16 bands of the γ -system ($A^3\phi - X^3\Delta$) have been analysed up to $v' = 5$, $v'' = 6$. When vibrational and rotational constants were calculated additional constants for higher order terms had to be included. The infrared spectrum of ZrO shows several bands between 8786 cm^{-1} and 10309 cm^{-1} . Identifications are under way. The well known 9290 Å band consists probably of three Q branches of a predicted triplet system. The 8192 Å band has been resolved into three branches belonging to a doublet system, presumably of ZrO^+ . A laboratory source enhancing the abundance of ZrO^+ is being developed.

2. Lifetimes and Absolute Transition Probabilities

TiO: A tunable dye laser has been used to measure the lifetime of the $C^1\phi$ state. Our results on the intercombination transitions ($C^3\Delta_3 - a^1\Delta_3$) agree with those of Broida and Linton, but we have problems to explain the anomalously weak P-line. Further intercombination emissions are being sought. For the α -system of TiO ($C^3\Delta_3 - X^3\Delta_3$) the radiative lifetime of two rotational levels of $v' = 2$ ($C^3\Delta_3$) has been measured by laser-induced fluorescence and delayed coincidence. The results are $\tau = 28.21 \pm 0.15 \text{ nsec}$ for $J' = 17$, and $\tau = 29.74 \pm 0.86 \text{ nsec}$ for $J' = 87$. Ar - TiO collision cross-sections for the two levels have been determined to differ by 30%. **ZrO:** We have recently (May 1978) collected data on the lifetime of the $B^3\Pi$ state using observations on the $\beta(B^3\Pi - X^3\Delta)$ system.

D. *From the Centre for Astrophysics, Harvard College Observatory* (Reported by W.H. Parkinson and J.L. Kohl)

The Atomic and Molecular Physics Division of the Harvard-Smithsonian Center for Astrophysics is engaged in quantitative studies of basic atomic and molecular processes having applications to astrophysical problems. A variety of experimental techniques and instruments are used to study atomic autoionization, photoionization, spectral lines broadening and radiative bound state transitions. A new Ion-Beam Facility was recently built to study the interaction of multiple charged ions with other particles and radiation fields, and the Division recently acquired a 6.6 meter evacuable spectrograph for quantitative measurements of molecular spectra and structure. The experimental work is closely associated with theoretical studies of atoms and molecules by the Center's Theoretical Atomic and Molecular Physics Group (208, 209, 210, 211, 212).

E. *From the Cavendish Laboratory, University of Cambridge* (Reported by A.H. Cook)

Molecular spectroscopy in the Laboratory Astrophysics group is undertaken with the aim of contributing to the understanding of maser action in astrophysics. A research student (J. Viney) has observed the pure rotation spectrum of OH using a Fourier transform far-infra-red spectrometer at the National Physical Laboratory and has detected transitions between the ${}^2\Pi_{3/2}$ and ${}^2\Pi_{1/2}$ series as well as transitions within each series. Mr. Viney has also used the synchrotron source and associated far ultraviolet spectrograph at Bonn to look for the ultraviolet spectra of molecules of astrophysical interest. He has seen spectra almost certainly to be attributed to Rydberg series of SiO (a molecule which shows maser action) and he has observed a sequence of broad bands very probably to be attributed to OH. These observations lie in the range 70-100 nm.

F. *From the Centre for Research in Experimental Space Science,
York University, Toronto*
(Reported by R.W. Nicholls)

The multifaceted experimental and theoretical research programme to provide absolute transition probability data and structure constants for astrophysical molecules continues, see also (4). Recommendations have also been made for consistent definitions of transition moments and line intensity factors for molecular spectra (15). A programme of high resolution shock tube spectroscopy and radiometry continues to provide transition probability data on C₂ (213), ScO (214), TiO, WO and ZrO. The same equipment provides high resolution spectra for band analyses of YO (215), WO and ZrO. High resolution photoelectric studies of CN have been interpreted by the method of synthetic spectra to provide transition probability data for the Violet (216) and Red Systems. Medium resolution (217) and high resolution measurements have been made of the absolute absorption coefficients of the ClO (A²Π - X²Π) bands. Realistic computer syntheses of Cometary spectra have been compared with observed spectra to diagnose physical conditions in Comets (218). High resolution computer syntheses have also been made of atmospheric transmission (219,220). The same facility has been used to assess CO₂ line position data (221). Theoretical studies have continued on molecular transition probabilities. Band strengths of the IR vibration-rotation bands of ClO have been calculated (222) and model studies have been made on the r-centroid approximation (223) and of photodissociation processes.

G. *Other Laboratories*

Lindgren has provided a set of extensive annual reports on the large research programme on diatomic molecular spectroscopy at Stockholm, some of which is devoted to astrophysical molecules and is referenced above. Leach provided reprints from an extensive research programme on diatomics and polyatomics in his Laboratoire de Photophysique (Paris), some of which are referenced above. Judge provided an extensive reference and reprint list of the research programme on vacuum UV photo-fluorescence studies at the University of Southern California.

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