

COMMISSION 14: ATOMIC AND MOLECULAR DATA (DONNÉES ATOMIQUES ET MOLÉCULAIRES)

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General

The rapid expansion during the past few years of the spectral region accessible to astronomical observers, from gamma rays to the radio region, has resulted in a corresponding expansion of the need for a wide variety of atomic and molecular data. Included are needs for accurate wavelengths, atomic and molecular energy levels, and transition probabilities. The continually improving resolution that has been attainable has resulted in the requirement of improved insight into line broadening mechanisms of various types. This expansion has placed an increasing premium on data compilation and dissemination, so that available information can be made readily available to potential users. Among the numerous compilations that have appeared might be mentioned the important National Bureau of Standards Bibliography on Atomic Levels and Spectra, which is up-dated periodically via successive supplements, and the NBS compilation and bibliography by the Data Center on Atomic Transition Probabilities. Several compilations or bibliographies on collision cross-sections are now available, such as that published by the Information Center at JILA. In the field of molecular spectra there has appeared the very comprehensive "Constants of Diatomic Molecules" by Huber and Herzberg. Other useful compilations are referred to in the reports of the five Working Groups that appear below.

WORKING GROUP 1: WAVELENGTH STANDARDS

The Primary Standard and the Rydberg

The present situation as regards the primary standard may be summarized as follows: the International Metre is officially based on the 606 nm wavelength of  $^{86}\text{Kr}$ , reproducible to about  $2 \times 10^{-9}$ . More reproducible wavelengths emitted by lasers stabilized on lines of  $\text{I}_2$ ,  $\text{CH}_4$  and  $\text{CO}_2$  are known to about the same uncertainty and can be considered equivalent to the primary standard. The frequencies of the  $\text{CH}_4$  and some of the  $\text{CO}_2$  lines are known in terms of the Cs primary standard of frequency to better than  $10^{-9}$ . The resulting calculated value for the speed of light ( $c = 299792458 \text{ m s}^{-1}$ ) has been adopted as the best value by the International Committee of Weights and Measures, with the recommendation that in any future re-definition of the metre, or of the second, this value should be unchanged and should be considered as exact. This is equivalent to an unofficial definition of the metre in terms of the speed of light and the second. In all probability such a definition will be formally adopted by the General Conference of Weights and Measures in 1983 but this depends on agreement on such matters as wording, adequacy of data and suitability of practical comparison techniques to ensure that the redefinition will provide a new more precise and widely reproducible standard, without significant discontinuity in the value of the metre. These questions will be considered during 1982 at meetings of the International Committee of Weights and Measures and its appropriate advisory committees: it now appears likely that the new definition will be in terms of the distance light travels in  $1/299792458$  seconds.

New measurements of the Rydberg have been made by Lichten et al. (1) in the U.S. and Petley et al. (2) in Britain yielding  $109\,73731.521$  (11)  $\text{m}^{-1}$  and  $109\,737$

31.513 (85)  $m^{-1}$  respectively, in good agreement with one another but significantly higher than that of Hansch et al. reported in 1978.

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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 critical compilation and bibliographical work on transition probabilities. An extensive critical compilation (262 pages) has been completed for the three elements Fe, Co, and Ni (1), which covers all stages of ionization on which reliable data are available. Also, a table of transition probabilities for about 5000 selected lines of all elements for which reliable data were available on an absolute scale was recently published (2). Work is now in progress on the updating and revision of the existing NBS critical data compilations for all allowed (1,3,4) and forbidden (5) transitions in Fe-group elements. A single volume containing all these data for the Fe-group elements Sc to Ni (Vol. III of the NBS series of atomic transition probabilities) is planned for publication in the 1982-1983 period. A new supplemental bibliography has been published, covering the literature references from November 1977 through March 1980 (6). It contains approximately 600 references in chronological order and includes listings by element, stage of ionization, and experimental or theoretical method applied, as well as an author index.

Below, the most recent literature references covering the period since the publication of our last supplement (March 1980) up to the present (August 1981) are listed (refs. 7-198), ordered alphabetically according to authors. Each reference contains some code letter(s), indicating the method(s) applied by the author. Specifically, the code letters are defined as follows:

#### THEORETICAL METHODS:

- Q - quantum mechanical (including self-consistent field) calculations.
- 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:

- C - additions or suggested revisions to data in previous articles, comments on particular theoretical or experimental methods, etc.
- Cp - data compilations.
- R - relative (non-absolute) oscillator strengths have been tabulated.

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

Also, in Table 1 the references are ordered according to element and stage of ionization. For brevity, the references are identified there only by the running number of the reference list.

Several groups have communicated their work in progress. At the Center for Astrophysics, Cambridge, Massachusetts, f-value measurements are in progress on Co I, V I and Si I. For Co I, the results of hook-method studies in absorption done at Cambridge are being combined with branching-ratio emission measurements carried out by W. Whaling, California Institute of Technology in order to provide data for 360 lines. For V I, a similar combined absorption-emission study is being carried out by the same researchers for approximately 210 transitions; this work is nearing completion. For Si I, oscillator strengths are being measured for about 70 lines in the range 1650 to 2000 Å by the hook method. Also, the principal intersystem transition of Mg I is being studied by the Cambridge group with a novel laser-excitation technique. R. Garstang of the Joint Institute for Laboratory Astrophysics, Boulder, has completed his work on Tc lines. At NBS, Washington, transition probability measurements in emission are under way for C I.

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TABLE 1

Selected references on atomic transition probabilities  
(numbers in parentheses correspond to references 7-198)

Ag I (49)	Cd II (49)	Ga I (134,198)
Al Sequence (73)	Cl Sequence (83)	Ga III (49,134)
Al I (72,103)		H Sequence (94)
Al III (49)	Co VIII (68)	He Sequence (93,105,113, 116,122,128,163,168, 169,172)
Al X (186)	Co XIX (132)	He I (39,45,82,171)
Ar I (8,15,32,34,56)	Co XX (132)	
Ar II (8,15)	Co XXI (132)	Hf IV (149)
Ar III (118)	Co XXII (132)	Hg II (49)
Ar V (135)	Co XXIII (132)	In I (130)
Ar VI (135)	Co XXIV (132)	In III (49)
Ar VII (135)	Co XXV (132)	
Ar VIII (135)	Cr I (103,191)	K Sequence (120)
Ar IX (116)	Cr II (95,191)	K I (10,49,109,150,164)
	Cr XVI (70)	Kr I (32,56)
Au I (49)	Cr XVII (70,132)	Kr XXXV (161)
B Sequence (48,65,66, 156,165,188)	Cr XVIII (70,132)	
B I (52,53)	Cr XIX (70,132)	Li Sequence (48,119,120, 156,165,167,168,177)
B II (138)	Cr XX (70)	Li I (21,35,43,49,50,80, 114,140,152,164)
	Cr XXI (70)	Li II (76,140,160)
Ba I (13,77,115,124, 145,159)	Cr XXII (132)	Lu III (149)
Ba II (49,148, 157,180)	Cs Sequence (120)	Mg Sequence (11,116,195)
	Cs I (49,150)	Mg I (7,124,133,145)
Be Sequence (48,87, 116,131,143,147, 156,165,166,170, 173,195)	Cu I (49,126,197)	Mg II (49,133,146)
Be I (52,97)	Cu II (21,74)	Mg III (41)
Be II (76,125,141)	Cu X (68)	Mg IV (41,117,122)
	Eu I (148)	Mg V (41,117,122)
C Sequence (48,165)	Eu II (148)	Mg VI (117,122)
C I (52)	F Sequence (37,48,147, 156,165,170)	Mg VII (117,122)
C II (53,117,154)	F I (176,181)	Mg VIII (117,122)
C III (21,25,122)	F II (176)	Mg IX (185,186)
C IV (112)		Mg X (122,182,185)
C V (112)	Fe I (9,33,101,103)	Mg XI (185,186)
Ca I (12,57,103,123, 124,158,189,193)	Fe II (153)	
Ca II (49)	Fe X (58,117,139)	Mn I (24)
Ca VII (122)	Fe XI (117)	Mo I (61)
Ca IX (122)	Fe XII (117,122)	
Ca XI (58)	Fe XIII (117)	N Sequence (48,62,85, 156,165,170)
Ca XII (122)	Fe XIV (71,117)	N I (46,51,56,117)
Ca XIII (122)	Fe XV (29,30)	N II (59,107,117)
Ca XIV (122,129)	Fe XVI (42)	N III (53,117)
Ca XV (122,129)	Fe XVII (42,70,122)	N IV (64,122,194)
Ca XVI (122,129)	Fe XIX (42,70,122,132)	
Ca XVII (122,129)	Fe XX (31,129)	
	Fe XXII (88,89,144)	
	Fe XXIII (70,91)	
	Fe XXIV (132)	
	Fe XXV (161)	



Na Sequence (98,120)	S IX (117,122)	Zn Sequence (195)
Na I (49,103,150,183)	S X (117,122,186)	Zn I (21,127)
Na II (136)	S XI (117,122,186)	Zn II (49,111)
	S XII (117,122,186)	
Ne Sequence (11,86,121)	S XIII (186)	Zr I (103)
Ne I (32,36,47,56,102,190)	S XIV (122)	Zr II (103, 162)
Ne II (117)		
Ne III (117)	Sb I (100)	
Ne IV (117)		
Ne V (16,117)	Sc I (179)	
Ne VI (117,122)		
Ne VII (92,194)	Si I (19,22,81)	
Ne VIII (122)	Si II (19,72,117,178)	
	Si III (18,19)	
Ni I (23,104,110)	Si IV (19)	
Ni IX (68)	Si V (122)	
Ni X (122)	Si VI (117,122)	
Ni XII (38,122)	Si VII (117,122)	
Ni XIII (38,122)	Si VIII (117,122,187)	
Ni XIV (38,122)	Si IX (117,187)	
Ni XV (38,122)	Si X (117,122,187)	
Ni XVI (122)	Si XI (186)	
Ni XVII (29,30,122)	Si XII (122)	
Ni XIX (122)		
Ni XX (70,122)	Sr I (124)	
Ni XXI (70,122,132)	Sr II (49)	
Ni XXII (70,122,132)		
Ni XXIII (70,122,132)	Ti I (14,108)	
Ni XXIV (70,122,132)	Ti II (55)	
Ni XXV (70,122)	Ti III (20,21)	
Ni XXVI (122,132)	Ti IV (20,60)	
Ni XXVII (122)	Ti V (20,60)	
	Ti VI (60)	
O Sequence (48,165,170)	Ti VII (60)	
O I (56,117)	Ti XIV (28)	
O II (63,69,117,151,196)	Ti XV (28)	
O III (17,79,117,155,175)	Ti XVI (28,129)	
O IV (53,78,117,174)	Ti XVII (28)	
O V (25,64,90,106)	Ti XVIII (28)	
O VII (75)	Ti XIX (28)	
	Ti XX (28)	
P Sequence (84)		
P III (40,72)	Tl I (134)	
P IV (99)	Tl III (134)	
P IX (184)		
P X (184)	V II (96)	
P XI (67,184)	V VII (38)	
P XII (67,184,186)	V VIII (38)	
	V IX (38)	
Rb Sequence (120)	V X (38)	
Rb I (49,137,142,150)		
	Xe I (32,56)	
S I (54,176)	Xe II (180)	
S II (117,176)		
S III (117)	Y I (44)	
S IV (26,27,72,117)	Y II (162)	
S V (192)		
S VII (58,99)	Yb II (149)	
S VIII (117,122)		

W.L. Weise  
Chairman of Working Group

## WORKING GROUP 3: COLLISION CROSS SECTIONS AND LINE BROADENING

A. Line Broadening

The most recent state of advances in the subject can be found in the 1980 Proceedings of the 5th International Conference on Spectral Line Shapes<sup>(1)</sup>. In<sup>(2)</sup>, Breene has reformulated basic theories of line broadening in a modern point of view. Review papers have been written: in<sup>(3)</sup> the emphasis is upon atomic lines broadened by electron and positive ions but some neutral atom broadening is discussed; <sup>(4)</sup>-<sup>(16)</sup> concern neutral atom broadening and the related topic of the interatomic potential.

1. Stark Broadening of Hydrogen or Hydrogenic Lines

Concerning the center of hydrogen lines, the difficult problem of ion dynamics (colliding ions are neither "impact" nor "quasi-static") dominates the actual preoccupations (<sup>(1)</sup>pp. 3-102, <sup>(7)</sup>, <sup>(8)</sup>). A comprehensive discussion of the underlying physics supporting the model microfield method (M.M.M.) has been done<sup>(9)</sup> and different model microfields have been used in calculations<sup>(10)</sup>. Three effects of ion dynamics have been displayed<sup>(11)</sup>. A numerical simulation has been performed<sup>(12)</sup> and the results agree within 10% with the M.M.M. Correlation effects between Doppler and Stark broadening have also been suggested<sup>(13)</sup>. New experiments testing ion dynamic effects have been performed ( $H_{\alpha}$   $H_{\beta}$   $H_{\gamma}$ ) for the whole profiles<sup>(14-17)</sup> and for the shifts<sup>(18)</sup> ( $H_{\alpha}$ ,  $D_{\alpha}$ : no effect in that case).

In fact the inclusion of ion dynamics in the theories has greatly reduced but not eliminated all the observed differences. For explaining the remaining discrepancies, a model has been proposed which includes effects from electron producing low-frequency fields and has been applied to  $Ly_{\alpha}$ <sup>(19)</sup> and  $Ly_{\beta}$ <sup>(20)</sup> with equally satisfactory agreement with experiment<sup>(21)</sup>. Impact theories have been found to be correct for  $H_{\alpha}$  fine structure transitions at very low densities ( $10^8 - 10^{11} \text{ cm}^{-3}$ ).

Concerning the wings of hydrogen lines, attention has been directed towards the satellite structures which appear as superimposed on the line profile: the role of hydrogen molecular lines has been evinced experimentally for  $H_{\beta}$ <sup>(23)</sup> and improved calculations, including  $H_2^+$  molecular potential, have been provided for  $Ly_{\alpha}$ <sup>(24)</sup>.

The contribution of electron collisions to the wings of  $H_{\beta}$  have been calculated with the dipolar exact resonance quantum theory<sup>(25)</sup> and the derived asymmetry is in agreement with earlier experiments.

Hydrogenic ion line profiles have been studied, especially in view of spectroscopic diagnostic in very dense and hot plasmas (<sup>(1)</sup>p. 295-432 and 153-166). An exact quantum analytic solution of the problem of line broadening for hydrogen like ions by electrons has been obtained in the dipole approximation<sup>(26)</sup>. Measurements of polarization shifts have shown the insufficiency of previous theoretical estimates<sup>(27)</sup>. Effects of fine structure splitting have been studied<sup>(28,29)</sup>. An impact theory of spectral line broadening has been developed for transitions between degenerate states and for anisotropic collisions<sup>(30)</sup>.

2. Stark Broadening of Overlapping Lines of Helium

Ion dynamics are also important and have been taken into account in two ways<sup>(31,32)</sup> and the M.M.M. gives the best agreements with the experiments<sup>(33-36)</sup>. Effects of molecular  $He_2$  structure have been detected in the wings<sup>(37)</sup>. For stellar spectra studies, improved M.M.M. line profiles have just been provided<sup>(38)</sup>.

3. Stark Broadening of Isolated lines

No revolutionary results have been obtained during that period, but a number of

new data of astrophysical interest have become available: impact and semi-classical (S.C.) or semi-empirical (S.E.) theories have been applied and numerous experiments (E) have been performed (Table I). Attempts are made for providing simple but reliable formulae, especially for higher ionization stages<sup>(1)</sup>pp. 191, 211, (40), (47), (51)), but also for neutral emitters<sup>(60)</sup>. One can point out the first observations of ion dynamic effects in helium isolated line profiles consistent with calculations based on an adiabatic unified theory for ion perturbers<sup>(35)</sup>. A detailed comparison between quantum and semi-classical calculations has been made on the example of Li I 2s-2p, evincing the break down at very low temperatures of the validity of the semi-classical treatment as expected<sup>(42)</sup>. j-l coupling has been introduced for lines of heavy elements showing departures from L.S. coupling<sup>(61)</sup>. Improvements to straight path S.C. theory has been proposed, taking classically into account the back reaction of the neutral emitter on the perturbing electron<sup>(62)</sup>. Systematic trends in Stark widths of isoelectronic sequences have been examined<sup>(63)</sup>, (1)p. 241). An attempt to predict the line broadening of autoionizing levels by electric fields has been elaborated and applied to A I<sup>(1)</sup>p. 281).

#### 4. Line Broadening by Foreign Gases and Resonance Broadening

A great deal of attention has been paid to atomic line broadening<sup>(1)</sup>pp. 593-757) and to related topic of excimers<sup>(1)</sup>pp. 767-826). Recent experimental and theoretical data concerning the impact broadening and shift of atomic lines broadened by the perturbers of astrophysical interest, atomic hydrogen<sup>(67)</sup>,<sup>(68)</sup> or helium<sup>(67)</sup>,<sup>(69)</sup>-(82) are collected in Table 2; <sup>(84)</sup> concerns high pressure non impact results, and <sup>(85)</sup>-(87) refer to molecular rotational or vibrational components and lines of OH and CO. The increased precision of the measurements of the two past years indicates many discrepancies of as much as 25% with the theory, evincing again the drastic influence of the interatomic potential. The different broadening of fine structure lines is generally well predicted and the effects of the various collisional coupling become to be very clearly understood<sup>(76)</sup>. Hyperfine structure effects have been shown for the first time<sup>(69)</sup>, leading to a collisional narrowing effect due to the H.F.S. decoupling at very low densities. In light of these considerations the simple formulae obtained in <sup>(88)</sup>,<sup>(89)</sup> for line broadening by neutral hydrogen must be used with caution, since the interatomic potential used takes only into account the overlap of the atomic charge distribution and neglect shorter range interactions which should be important.

The numerous works<sup>(1)</sup>pp. 827-866) which concern resonance broadening are not reported here, since their interest is far from direct astrophysical applications. The same remark concerns the topic of excimers: it is a very exciting branch of the study of line profiles and extreme line wings in connection with the asymptotic behaviour of the interaction potential of the quasimolecule formed during the collision. The interaction of these collisional processes with the absorbed and emitted radiation processes brings us to the last part of the report. We will quote only <sup>(90)</sup>,<sup>(91)</sup> for showing the future importance of these processes for high resolution spectroscopy of astrophysical spectra.

#### 5. Collisional Redistribution of Radiation and Related Phenomena

Recent developments in high resolution and high power laser sources have resulted in an increased interest in collisional redistribution of radiation. Astrophysical needs remain numerous and will certainly profit of these progresses. Previous work on the redistribution of weak (excitation may be considered as an independent scattering of separate photons) radiation due to collision, has been extended to situations in which absorption or emission of radiation can occur in the non impact (line wings) of the spectrum<sup>(92)</sup>,<sup>(93)</sup>. It has been shown that inelastic collisions may well redistribute the radiation<sup>(94)</sup>-(96). The effect of correlations between radiative and collisional events has been included in a consistent way by

Table I

STARK BROADENING OF ISOLATED LINES

Lines	Références	Range of plasma parameters ( $N_e$ cm <sup>-3</sup> , $T^\circ$ K)
He I (12 lines)	(35) E	$0.2-1.3 \cdot 10^{16}$ , $1.-2 \cdot 10^4$
He I 6678, 5876, 3889	(36) E	$10^{17}-2 \cdot 10^{18}$ , $1.-2 \cdot 10^4$
He I 3965	(39) E	$1.3-1.9 \cdot 10^{16}$ , $1.5 \cdot 10^4$
He I (12 lines and 42 lines)	(40) S.C.P.	- , $2 \cdot 10^4$
Alkali resonance lines	(41) M.M.M.	$10^{17}$ , $2 \cdot 10^4$
Li I 2s2p	(42) S.C.P., C.C.	- , $2.5 \cdot 10^3-2 \cdot 10^4$
Fe I 5383	(43) E	$7 \cdot 10^{15}$ , $10^4$
Ni UV (15 lines)	(44) E	$4 \cdot 10^{16}-3.7 \cdot 10^{17}$ , $1.1-1.5 \cdot 10^4$
NII/III/IV (13 lines)	(45) E, (40) S.C.P.	$1.4 \cdot 10^{18}$ , $5 \cdot 10^4$
108 lines from doubly and triply ionized atoms from Be to Ar	(1) P 212-239, (41), (59) S.E., S.C.	- , $10^4-8 \cdot 10^4$
CII UV	(66) E	
S III/IV (17 lines)	(48) (53) E, S.E.	$5.1 \cdot 10^{16}$ , $2.8 \cdot 10^4$
Alkali like ions	(49) S.E.	
Mg I 2852, Mg II 2795	(50) E	$1.1-1.6 \cdot 10^{17}$ , $1.3-1.4 \cdot 10^4$
Al I (4 lines)	(65) E	$1.5-6 \cdot 10^{16}$ , $1.2 \cdot 10^4$
O II/ III (17 lines)	(51) S.E. (52) S.C.	$10^{17}$ , $2 \cdot 10^4$ , $5 \cdot 10^{16}$ , $2.5 \cdot 10^4$
Ar I 3949	(58) E	$1.5-5 \cdot 10^{16}$ , $1.2 \cdot 10^4$
Sn I 5p-6s, Sn II (10 lines)	(54) E, (55) S.E.	$5-12 \cdot 10^{16}$ , $0.9-1.2 \cdot 10^4$
Bi I (3 lines)	(56) E	$4-12 \cdot 10^{16}$ , $1-1.2 \cdot 10^4$
Pb I /II (8 lines)	(57) E	$5-13 \cdot 10^{16}$ , $1.1-1.2 \cdot 10^4$
Xl I (8 lines)	(58) E	$2.2-10 \cdot 10^{16}$ , $0.9-1.2 \cdot 10^4$

E = Experimental. T = Theory; Q = Quantum, B = Born, S.C. = Semi-Classical,  
P = Perturbation theory, C.C. = Close Coupling, M.M.M. = Model Microfield Method,  
S.E. = Semi Empirical.

Table II COLLISIONAL BROADENING BY FOREIGN GASES

<u>Lines</u>	<u>References</u>	<u>Density (cm<sup>-3</sup>), Temperature (°K)</u>
Na I D <sub>2</sub> + H and He	(67) E	3.6-12 10 <sup>19</sup> , 5-10 10 <sup>3</sup>
H <sub>α</sub> + H	(68) E	4.10 <sup>19</sup> , 10 <sup>4</sup>
H <sub>α</sub> (fine structure lines) + He	(69), (70) E	0.7-3.5 10 <sup>16</sup> , 310
He I (2p <sup>3</sup> P <sub>0</sub> - 3d <sup>3</sup> D <sub>1</sub> ) + He	(71) E	
Na D <sub>1</sub> and D <sub>2</sub> + He	(72) C.C., (74) E, (75) E	—, 500-2000; 10 <sup>17</sup> -10 <sup>19</sup> , 450
K 4s-5p (f.s. lines) + He	(76) Q, S.C., C.C.	1-6 10 <sup>18</sup> , 450
K 4p-7s (f.s. lines) + He	(77) E	3-10 10 <sup>17</sup> , 450
K 4s-4p + He	(82) E	5-15 10 <sup>18</sup> , 400
Rb (Rydberg states) + He	(78) E	0.6 10 <sup>16</sup> -10 <sup>17</sup> , 463
Rb (D <sub>2</sub> ) + He	(79) (E)	
Fe I (42 lines) + He	(81) E	up to 10 <sup>19</sup> , 2000
Ca I (mult. 3) + He	(80) (E)	up to 10 <sup>19</sup> , 2000
Ca I 4227, Ca II H, K, 8542, 8662 + He	(81) E	10 <sup>18</sup> , 520-800
Mg I/II, Ca I/II, Sr I/II (F.S. lines) + He	(1) p 733, E	
Cs I (8p-6s) + He	(84) E, unified theory	10 <sup>19</sup> -5.10 <sup>21</sup> , 478
Al I + He (4 lines)	(83) E	1.5-5 10 <sup>19</sup> , 1350
O H X <sup>2</sup> Π <sub>3/2</sub> ( <sup>3</sup> / <sub>2</sub> → <sup>5</sup> / <sub>2</sub> ) + He	(85) E	2 10 <sup>16</sup> -10 <sup>17</sup>
C O + H <sub>2</sub>	(86) E, Q, C.C.	10 <sup>15</sup> , 300
C O + H <sub>2</sub> and He (v = 0 → v = 1)	(87) E	10 <sup>17</sup> -10 <sup>19</sup> , 100,300

using the density matrix formalism<sup>(97)</sup> and has been extended to degenerate atomic systems<sup>(98)</sup> outside the impact limit<sup>(99)</sup>. Explicit expressions have been derived for the frequency distribution in the wings of  $\text{Ly}_\alpha$ <sup>(100)</sup>. Radiative transfer equations have been rederived<sup>(101)</sup>.

The case of redistribution of strong (stimulated emission rates become important) resonance radiation has also been studied<sup>(102)-(107)</sup>. Correlated events in which absorption of radiation during a collision and propagation to the final Zeeman states superposition at the end of the collision is important, have been considered, in order to explain, in particular, the polarization of light collisionally redistributed from the far line wings of atomic transitions<sup>(108),(109)</sup>.

This new topic of radiatively assisted inelastic collisions has a rapid development <sup>(1),(110)-(114)</sup> owing to its growing importance to the detailed study of the far wings of spectral lines and of the adjacent continuum.

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#### B. Collision Cross Sections

Data compilations or bibliographies are produced by the Information Center of JILA (University of Colorado and NBS), Institute of Plasma Physics (Nagoya University), Oak Ridge National Laboratory (Oak Ridge, Tennessee), and by the International Atomic Energy Agency (Vienna). A compilation on data relevant to gas lasers has been organized by E.W. McDaniel et al. for the U.S. Army Missile Research and Development Command (Redstone Arsenal, Alabama). Daresbury Laboratory (U.K. Science Research Council) issues an information quarterly about research on continuum states. An annual summary of atomic collision research in Japan is published by the Society for Atomic Collision Research (Tokyo). Summaries of recent activities may be found in the Abstracts and the Invited Papers and Progress Reports of the International Conferences on the Physics of Electronic and Atomic Collisions. The XIth was held in Kyoto, Japan, and the Abstracts were edited by K. Takayanagi and N. Oda. The XIIth was held in Gatlinburg, Tennessee and the Abstracts were edited by S. Datz. The Invited Papers and Progress Reports are published by North-Holland. *Advances in Atomic and Molecular Physics* (Academic Press) is an annual review, edited by Sir David Bates and B. Bederson. The book, *Atom-Molecule Collision Theory* (Plenum Press), edited by R.B. Bernstein, appeared in 1979. Sir Harrie Massey, B. Bederson and E.W. McDaniel are editing a series of volumes on Applications of Atomic Collision Physics to be published by Academic Press, and Cambridge University Press is to publish a book "Rydberg States of Atoms and Molecules" edited by F.B. Dunning and R.F. Stebbings.



Most of the papers on collision cross sections appear in the Journal of Physics B, the Journal of Chemical Physics, Physical Review A, Chemical Physics Letters and Chemical Physics.

## 1. Heavy Particle Collisions

Because of the size and diversity of the material on heavy particle collisions, I give references only to those of immediate relevance to astronomical research.

### 1.1 Ion-molecule and Neutral Reactions

Lengthy tabulations of the rate coefficients of reactions occurring in the interstellar gas and in cometary atmospheres have been presented by Schiff and Bohme [1], Prasad and Huntress [2], de Jong et al. [3], Huntress et al. [4], Hennings [5], and Graedel et al. [6]. Hartquist et al. [7] and Hollenbach and McKee [8] have compiled lists of rate coefficients of reactions occurring in shocked gases. Numerous related laboratory measurements have been reported. For ion-molecule reactions see [9-23] and for neutral reactions [34-50]. Theoretical work is more limited and is concentrated mostly on radiative association reactions [51-57], though the relative stability of  $\text{CNC}^+$  and  $\text{CCN}^+$  has been calculated [58] and the effects of departures from equilibrium on reaction rates have been explored [59]. Collision frequencies of ions with polar molecules have been computed by Sakimoto and Takayanagi [59]. Formation mechanisms of molecules on grain surfaces has been examined in a few papers [62-65].

Proton impact excitation is important in astrophysics usually in connection with fine-structure excitations. Calculations of rate coefficients for beryllium-like ions of N, O and Ne have been reported [66] as have rate coefficients of carbon-like ions of N, O, Ne, Na and Mg [67]. Various ionization stages of Ca, Fe and S have also been studied [68]. Charge transfer recombination and ionization processes can greatly modify the ionization structure of astrophysical plasmas. Rate coefficients for doubly and trebly-charged ions of most astrophysically interesting elements have been calculated [69-78] and measurements at thermal energies have been published for charge transfer with helium [79-81]. Values have also been derived empirically from analyses of nebulae [82]; some differences persist [83,84]. Charge transfer of singly-ionized carbon and sulphur with hydrogen has been studied [85] and detailed results have been obtained for the important cases of  $\text{O}^+$  in H [86] and of  $\text{O}^+$  in D [87, 88].

Cross sections for the rotational excitation of heteronuclear molecules in collisions with  $\text{H}_2$  and with He are needed for the interpretation of molecular spectral line observations in the radio region. Of particular importance are collisions of CO. For He-CO collisions see [85-95].  $\text{H}_2$ -CO collision cross sections are frequently obtained by simply scaling the He-CO interaction. A calculation of the  $\text{H}_2$ -CO potential energy surface has been reported [96]. For other interstellar molecules see [97-101]. Rotational excitations by collision with positive ions has been investigated by Sakimoto [102].

Rotational and vibrational excitation of  $\text{H}_2$  in direct and reactive collisions with H, He and  $\text{H}_2$  occur in interstellar clouds and in shocked regions of the interstellar gas. Many studies have been made of various aspects of the collision processes [103-123] though a comprehensive account is not yet available. Collision-induced dissociation, an important mechanism in rapid shocks, has been investigated and approximate estimates are available for  $\text{H}_2$  and for CO [124,125].

Cross sections for collision-induced transitions of the masing molecules by collisions with H and  $\text{H}_2$  have received some attention since the last report. For OH, see [126-129], for  $\text{H}_2\text{O}$  see [101] and for SiO see [130]. Charged particle excitation of OH has been investigated by Bouloy and Omont [131] and Elitzur [132].

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#### WORKING GROUP 4: STRUCTURE OF ATOMIC SPECTRA

##### A. Laboratory Results

A Bibliography on Atomic Energy Levels and Spectra covering the research literature from July 1975 through June 1979 is now available (1). A selection of references for the period after June 1979 is given in Table 1, with the reference numbers (2-93) sorted according to spectrum. These references are with few exceptions limited to new data on energy levels, wavelengths, and line classifications. The citations for  $Z > 28$  were selected from papers on the first five spectra only.

##### B. Compilations and Predictions

A continuing strong interest in high-ionization spectra, evident in Table 1, is also apparent in recent compilations of such data. Indeed, several papers listed in

Table 1 include, in addition to original data, more or less extensive compilations of related data on highly ionized species. Lawson and Peacock, for example, give wavelengths and levels for XUV transitions involving the basic  $2s^m 2p^k$  ( $m = 2, 1, 0$ ) configurations in ions of the elements Cr to Ni (53) (see (78) also). Similar data for the elements Ar to V are listed by Fawcett et al. (56). Eidelsberg et al. have compiled experimental and predicted wavelengths for forbidden lines from hot astronomical sources ( $250 \text{ \AA} - 10 \text{ \mu m}$ ) (77).

Edlen has continued his compilations and predictions of energy levels of the  $2s^m 2p^k$  ( $m = 2, 1, 0$ ) configurations along isoelectronic sequences with recent papers on the F I-, O I-, and Be I-like spectra (94) and on the B-like spectra (95). He is working on a similar treatment of the C I sequence. The wavelengths of transitions involving  $1s$ -excitations in Be I-like spectra ( $1s^2 2s^2 - 1s 2s^2 2p$ , etc.) are included in the quantities calculated by Safronova and Lisina for  $Z = 6, 8, 10-42$  (96). Calculated wavelengths for the  $1s^2 \ ^1S_0 - 1s 2s \ ^3S_1$  and  $1s^2 \ ^1S_0 - 1s 2p \ ^3P$  lines in the He I isoelectronic sequence are given by Safronova for  $Z = 10-42$  (97). The series formulae given by Martin for the spectra Na X through Ar XVII ( $Z = 11-18$ ) in the He I sequence are equivalent to energy-level and wavelength predictions for all transitions in these ions (98).

Since 1979 the NBS Atomic Energy Levels Data Center has published new critical energy-level compilations for all spectra of ten elements: Na I-XI (99), Mg I-XII (100), Al I-XIII (101), K I-XIX (102), Ca I-XX (103), Sc I-XXI (104), Ti I-XXII (105), Fe I-XXVI (106), Co I-XXVII (107), and Ni I-XXVIII (108). A single volume of atomic energy-level data covering the iron group K through Ni ( $Z = 19-28$ ) is being prepared as a collection, with additions and revisions, of the recently completed compilations for the 235 spectra of these elements. A new compilation of the levels for the Si spectra is also under way. C.E. Moore has published her compilation of the energy levels and multiplet tables for O V (109) and O IV (110) and plans to complete these Selected Tables of Atomic Spectra with the data for O III and O II.

TABLE 1

Selected references on energy levels and line classifications  
(supplementary to reference (1))

He I (48,89)	Ca I (16,41,72)	Fe XXIII (3,8,30,53,71)
Li I (22,63)	Ca XIV,XV (56,77)	Fe XXIV (3,8,30,53,76)
Be II (59,75)	Ca XVI-XVII (56)	Fe XXV (3,79)
Be III (31,75)	Ca XVIII (56,76)	
C I (39,64)	Sc II (5)	Co VII (85)
C IV,V (49)	Sc XV-XVIII (56)	Co VIII (26)
	Sc XIX (56,76)	Co IX (57)
N III (45)	Ti II (92)	Co XI-XV (25)
O I (20)	Ti XII (5)	Co XI-XV (25)
O IV (36)	Ti XIV,XV (21,69,78,87)	Co XVI (11,25)
O V (46,88)	Ti XVI (56)	Co XVII (25,53)
O VI (36)	Ti XVII (21,56,69,78,87)	Co XVIII (30,33)
O VII (9,36)	Ti XVIII (56,69,78,87)	Co XIX (4,30,33)
	Ti XIX (56,78)	Co XX (30,33)
Mg V (43)	Ti XX (56,76)	
Mg IX (35,77)	V XII (11)	Ni V (70)
Mg X (15,35,76)	V XVII-XX (56)	Ni VI (38,70)
Mg XI (35)	V XXI (56,76)	Ni IX (26,34)
		Ni X (34,57)
Al VI (40)	Cr IX (77)	Ni XI (34)
Al X (35)	Cr XIII (11)	Ni XII (25,34)
Al XI (6,15,35,76)	Cr XIV (53)	Ni XIII-XVII (25)
Al XII (35,60)	Cr XVI (30,53,93)	Ni XVIII (25,53)
	Cr XVII (53,93)	Ni XIX (30,33,53)
Si II (74)	Cr XVIII (30,53,93)	Ni XX (4,30,33,53,87)
Si XII (76)	Cr XIX (53,87,93)	Ni XXI (30,33,53)
Si XIII (18)	Cr XX (2,53,87)	Ni XXII (2,53)
	Cr XXI (30,53)	Ni XXIII (2,53,87)
P XI-XIII (76)	Cr XXII (30,53,76)	Ni XXIV (2,30,53)
	Cr XXIII (30)	Ni XXV (8,53)
S III (80)	Mn VI (91)	Ni XXVI (8,30,53)
S IV (32)	Mn VII (57)	
S V (82)	Mn XIV (11)	Cu I (19)
S VI (10)	Mn XV (53)	Cu IV (44)
S XIV (76)	Mn XVII-XIX (53)	Cu V (67)
S XV (18)	Mn XX-XXII (13,53)	
	Mn XXIII (53,76)	As IV, V (84)
Cl VIII (90)		Kr IV, V (37)
Cl XV (76)	Fe V,VI (70)	Zr III (83)
Cl XVI (18,52)	Fe VII (65)	Zr IV (28,54)
	Fe VIII (57)	
Ar VII (66)	Fe XIV (77)	Cd III (51)
Ar XV (56)	Fe XV (23)	Cd IV (29)
Ar XVI (6,56,76)	Fe XVI (53)	
	Fe XVII (30,33,55)	In I (27)
K XII-XVI (56)	Fe XVIII (4,30,33,53,87)	Sb I (12)
K XVII (56,76)	Fe XIX (30,33,53,87)	
	Fe XX (24,53,71)	I I (73)
	Fe XXI (53,71,93)	
	Fe XXII (30,53,71,87)	Cs I (17,50,58,68)

TABLE 1 continued

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Ba I (7,47)  
Pr I (81)  
Er I (61)  
Yb I (14, 62)  
Lu IV (86)  
Hf V (86)

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The new NSRDS-NBS volume of wavelength tables has about 47,000 lines (40–40,000 Å) from the first five spectra of all elements, arranged both by element and in a finding list (111). Varshni has prepared a new multiplet table for Fe III (112), and the Grotrian and energy-level diagrams for Fe VIII–Fe XXVI compiled by Mori et al. have been published (113). A new multiplet table for Fe II in the 1050–2200 Å region has been prepared by Johansson (114).

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## WORKING GROUP 5: MOLECULAR SPECTRA

A. Compendia. Bibliographies. Atlases.

Molecular Spectroscopic research over much of the electromagnetic spectrum, and its literature, has continued to proliferate strongly during the past three years, stimulated in part by the impact of laser methods on research programmes and the search for new molecular laser materials, and in part by the needs of diagnostic applications in environmental, atmospheric circumstances. The literature is so prolific that it is impossible to make a definitive review here even of that which is relevant to astrophysical needs from the microwave to the vacuum UV spectral regions. The trends and literature citations below have been compiled principally from reports received from individual workers and from Research Centres.

The bi-monthly Berkeley Newsletter (1) compiled by Phillips, Davis and Eakin from molecular spectroscopic publications in more than 30 journals continues to be a prime research bibliographic tool and is regularly circulated to more than 500 workers. The growth in its size is an indication of the explosive growth of the field referred to above. The average page run per issue was 23 in 1979 and is 31 in 1981. A recent single issue had about 700 individual citations.

Users of molecular spectroscopic data agree that a desperate need remains for critically assessed reliable basic data on spectra of importance to their work. Huber and Herzberg's important compilation of molecular data (2) is a major contribution to such needs for diatomic molecular spectra. CNRS has provided an important companion to Rosen's *Donnees Spectroscopique* in the publication of a critical bibliography of molecular spectral data (3). Lovas et al. (4) have published a critical compilation of characteristic microwave rest frequencies for important interstellar lines and molecular transitions. MacPherson and Barrow (5) have published an important review on gas phase molecular spectra.

A number of useful books have been recently published including those of Okabe (6) on photochemistry of small molecules, Berkowitz (7) on photoabsorption, photoionization and photoelectron spectroscopy, Slater (8) on the calculation of molecular orbitals and Bunker (9) on molecular symmetry and spectra.

B. Molecular Data

Over the past three years there has been a continuing emphasis in the literature on experimental and theoretical studies of the spectra of diatomic and small polyatomic molecules which occur in astrophysical, atmospheric and laser situations. The success of ab initio theoretical methods which incorporate self-consistent field and configuration interaction formalisms in matching experimental results for the spectra of light diatomic molecules is particularly gratifying. A recent example of such work, applied to infrared and ultraviolet bands of NO is that of Cooper (10). Astrophysical diagnostic applications of such spectra continue to call for high quality molecular structure and transition probability data for the species involved. The compilation of Huber and Herzberg (2) is an invaluable reference for molecular structure constants. There is also a continuing need for thermochemical information on many molecular species.

1. Electronic Band Analyses and Constants of Diatomic Molecules

Honjou et al. (11,12) have made ab initio theoretical studies on 6 of the electronic states of CaH. Linton et al. (13) have analyzed CeO spectra and located seven of the low lying states. Amiot et al. (14) have made a re-analysis of the C<sub>2</sub> Ballik-Ramsay system. Kotlar et al. (15) have made a very comprehensive re-analysis of the CN Red system to determine perturbations and deperturbed vibration-rotation constants for the A and X states. Unpublished tables of data relative to this work

are available. Harris and Barrow (16) in recent studies of the FeO spectrum have assigned 400 lines to 12 bands (which involve the ground state). Carroll reports continuing analyses of FeO spectra at University College Dublin. Bernard and Sibal (17) have performed a re-analysis of the spectrum of LaO. Matsumura et al. (18) report new structure constants for NS. Amiot et al. (19) have made new analyses of the IR OD spectrum from which new structure constants are derived. Coxon (20,21) reports continued studies of the IR, microwave and UV spectrum of OH from which definitive and consistent structure constants are derived. Balfour and Lindgren (22) have reanalyzed a band system of  $ZrO^+$ .

## 2. Transition Probabilities, Lifetimes, Intensities

Following discussion at the meetings of Commission 14 at the 1979 Congress of the IAU in Montreal, Whiting et al. (23) proposed uniform definitions for Honi-London factors and electronic transition moments of molecular band systems, which were endorsed. Huber and Sandeman (24) report a forthcoming review of oscillator strength measurements. Kendall and Clark (25) have measured absolute line strengths and integrated intensities for three OH submillimetre features. Clark and Kendall (26) have measured line strengths of  $O_2$  submillimetre magnetic dipole transitions. Cooper (10) has calculated IR band strengths and electronic transition moments for NO beta and gamma band systems. Thorne of Imperial College reports refractive index and Rayleigh scattering measurements in  $O_2$  in the ultraviolet. Kumimoto et al. (27) has determined band model parameters for  $SO_2$  IR bands. Osumi and Kumimoto (28) have determined line shape parameters for  $SO_2$  bands. Bass et al. (29) report studies of temperature dependence of UV absorption cross sections of atmospheric interest, specifically for  $O_3$ ,  $SO_2$  and  $CH_2O$ . Marr (30-35) reports continuing photoionization measurements of atmospheric molecules ( $N_2$ ,  $O_2$ , CO,  $H_2$  and  $CH_4$ ) using photoelectron spectroscopy and synchrotron radiation. Sampson (36-40) reports on photoelectron spectroscopic studies of vibrational intensity distributions of electronic states of  $O_2^+$ ,  $N_2^+$  and  $CO^+$ .

## 3. Polyatomic Molecules

Microwave and infrared measurements of  $CO_2$  constants have been made respectively by Endo et al. (40), Arcas et al. (41) and by Maillard et al. (42). Infrared measurements have been made on the  $4\nu_2$  band of  $H_2O$  by Camy-Peyret et al. (44). The dipole moment of  $HO_2$  has been measured by Saito et al. (45). Collision induced laser light scattering studies have been made on  $CH_4$ ,  $CF_4$  and  $SF_6$  to determine dipole-quadrupole and dipole-octopole polarizability tensors by Shelton et al. (46). The  $3\nu_3$  band of methane has been studied by Pierre et al. (47), and regions of weak methane absorptions have been studied by de Bergh et al. (48). New  $CH_3D$  bands of planetary interest have been reported by Lutz et al. (49). Microwave measurements have been made on  $CH_3OD$  by Kaushik et al. (50,51). Kojima (52) has made molecular structure measurements on  $CH_3SH$ . Tsunekawa et al. (53) report studies of the microwave spectrum of hydrazine ( $N_2H_4$ ), and Yamada et al. (54) infrared studies on the infrared spectrum of hydrazoic acid ( $N_3H$ ). Microwave structure constants of excited vibration states of acetylene-d have been made by Matsumura et al. (55). Structure constants of  $ClO_2$  have been measured by Hamada and Tsuboi (56).

## RESEARCH IN PROGRESS

### A. From the National Research Council of Canada (reported by G. Herzberg)

Spectroscopic studies of molecules of astronomical interest have continued to be one of the principal activities in this laboratory. A good deal of work on diatomic molecules has been done in the last three years. The work on the vacuum ultraviolet spectrum of  $H_2$  has been continued. Further studies of the dipole spectrum of HD have been made (61)(100). The pure rotation quadrupole spectrum of  $H_2$  has been observed

for the first time (70) as well as the quadrupole rotation-vibration spectrum of  $D_2$  (69). The ultraviolet and vacuum ultraviolet spectra of the hydrides NH (57)(62) and HCl and HF (80) have been studied and new electronic transitions have been found. For CaH a re-assignment of the ultraviolet spectrum has been made, and the predissociation of CH (75) has been further studied. Some information about SD has been obtained from laser magnetic resonance (96). The ground state constants of NO have been re-evaluated from a detailed study of the infrared spectrum (82)(85). The laser frequencies and Dunham coefficients for CO in its ground state have been considerably improved (77). The first observation of a spectrum of the FO radical was made by laser magnetic resonance and some of the constants of this molecule determined (87). The laser magnetic resonance spectra of ClO (97) and BrO (105) were studied. The first high resolution observation of a spectrum of TiN was made in the visible region (93). Only two diatomic ions were studied during the last three years, namely  $HeNe^+$  (66), already mentioned in the previous report, and  $HeAr^+$  (107).

A Rydberg spectrum of triatomic hydrogen was discovered in the visible and near infrared regions and analysed in detail (84)(92)(95)(103). In addition the rotation-vibration spectrum of  $H_3^+$  was observed and analysed for the first time (99). Laser magnetic resonance observations have greatly increased our knowledge of the ground state of  $HO_2$  and  $DO_2$  (63)(88) as well as DCO (104). The ground state constants of  $NH_2$ , NHD and  $NO_2$  have been studied, both by conventional absorption spectroscopy, and by laser magnetic resonance (71)(78)(86)(89)(91)(101). Improved constants of  $H_2O$  (76), of FNO (65),  $NO_2$  (94),  $HNO_2$  (98), and  $CH_2NH$  (73) have been obtained from laser Stark spectroscopy and radiofrequency double resonance. A considerable amount of work was done on various spectra of  $H_2CO$  and its isotopes (59)(60)(67)(68)(79)(81)(90) both in the infrared and ultraviolet. Laser excited fluorescence from single rovibronic levels in both  $H_2CO$  (72) and  $H_2CS$  (102) has been observed. For  $NH_3$  the transition dipole in excited vibrational levels has been determined (83). The ultraviolet and vacuum ultraviolet absorption spectra of  $N_2H_2$  have been re-examined (58)(106). Spectra obtained in various discharges through ammonia at high pressure, first observed by Schuster and by Schuler, Michel and Grun have been studied under high resolution, and conclusive evidence has been obtained that these spectra are Rydberg spectra of  $NH_4$  and  $ND_4$  (108). The 9613 Å band of  $CH_3D$  has been studied under high resolution (64).

#### B. From the National Bureau of Standards (reported by Frank J. Lovas)

The Molecular Spectroscopy Division of the National Bureau of Standards carries out molecular spectroscopy experimental studies in the microwave, infrared and visible regions and develops critical reviews on microwave spectra of interstellar molecules and tables of absorption lines for calibration of diode laser measurements.

During the past three years, seven new molecules have been completed for the series "Microwave Spectra of Molecules of Astrophysical Interest" published in J. Phys. Chem. Ref. Data (JPCRD). The species covered were propyne ( $CH_3CCH$ ) [109], methyl formate ( $HCOOCH_3$ ) [110], dimethyl ether ( $CH_3OCH_3$ ) [111], formic acid ( $HCOOH$ ) [112], methyl cyanide ( $CH_3CN$ ) [113], methane ( $CH_4$ ) [114], ethanol ( $C_2H_5OH$ ) and propionitrile ( $C_2H_5CN$ ) [115]. Approximately half of the known interstellar molecules have now been critically reviewed. A new series has been initiated in the infrared with the goal of providing absorption line standards for instrument calibration (principally diode lasers). The first publication on  $N_2O$  will appear in JPCRD in 1982 [116] and a second paper on OCS will be completed in the next year. A considerable effort to develop precise measurements on OCS was required as reflected in a number of publications [117-120]. Also high resolution measurements on SiO [121],  $SO_2$  [122],  $^{13}CO_2$  [15], and  $C_2H_6$  [16] have been completed.

Vibrational and electronic spectra of the free radicals CNC [125], CNN [126],

HCO [127], PO and HPO [128,129], and CH<sub>2</sub>OH [130] have been studied by matrix isolation techniques.

C. From the Center for Astrophysics, Harvard College  
Observatory and Smithsonian Astrophysical Observatory  
(reported by W.H. Parkinson)

Oscillator strengths for lines of simple molecules seen, or searched for, in diffuse interstellar clouds are being measured in the Atomic and Molecular Astrophysics Laboratory, Center for Astrophysics. Oscillator strengths have been measured by quantitative photographic methods with the 6.65m normal incidence vacuum spectrograph for lines of the 1240Å band of H<sub>2</sub>O (131), the (0,0) and (1,0) bands of the HCl system at 1290Å (132), and the 1150Å band of H<sub>2</sub>O at 1150Å (133). Oscillator strength measurements are in progress for 7 bands of H<sub>2</sub>CO between 3100 and 3550Å.

In 1980 the spectrograph, which operates between 600Å and 4000Å at a resolution of 0.007Å was fitted with a photoelectric scanner to permit absorption cross section measurements to be made between 1200Å and 4000Å at an instrumental band width of 0.013Å (134).

With this instrument absorption cross section measurements have been made for O<sub>2</sub> Schumann Runge bands (both more and less predissociated) between 1750Å and 2050Å. New high precision wavelength measurements of line center positions have also been made. High resolution absorption spectra of N<sub>2</sub> Rydberg bands between 885Å and 995Å have also been studied (135). Experiments are in progress to obtain high resolution photographic absorption spectra of pure O<sub>3</sub> in the 2100-3700 Å region of the Huggins and Hartley bands.

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

An extensive experimental and theoretical research programme continues for the provision of absolute transition probability data and structure constants for astrophysical molecules and applications. Increasing emphasis has recently been given to the application of such work to the study of high resolution extinction properties of molecular atmospheres in the ultraviolet (136,137) and in the infrared (138,139) through realistic numerical spectral syntheses based on reliable molecular data. Recommendations have been made for consistent definitions of line intensity factors and electronic transition moments (23). The shock tube spectroscopy programme continues (140,141). Nearly 100 new bands of WO have been discovered in the shock excitation of metatungstic acid (142). Revised absolute band strengths have been provided for AlO (143), and new molecular constants have been provided for NO (144). Studies at high resolution of the location and intensity distribution of ClO absorption band lines continues. Theoretical studies are also being made of the systematic properties of photodissociation continua (145). An approximation has been developed to provide simple formulae for Franck-Condon factors (146) for band systems for which molecular data are too sparse to allow realistic calculations to be made. This is often the case for band systems of astrophysical interest, for a number of which Franck-Condon factor arrays have now been provided (147), and the systematics of Franck-Condon factor arrays are being re-examined. A method has been suggested to improve the ultraviolet sensitivity of silicon photodetectors (148), and experiments are in progress to assess it. Diagnostic spectroscopic methods are being used to determine particle size distributions of atmospheric aerosols (149), and model studies are being undertaken on the spectral reflectance properties of minerals and rocks (150).

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REPORT ON SOVIET WORKS IN THE FIELD OF FUNDAMENTAL SPECTROSCOPIC DATA  
FROM 1978 to 1981

A. Atomic Data

1. Theoretical calculations of energy levels, transition probabilities, life-times for atoms and ions were performed. Using a charge-expansion perturbation approach with hydrogen-like wave-functions and relativistic Breit corrections many atomic constants for systems with 1-10 electrons were calculated (1-13). A model potential method based on Dirac equations was applied to obtain energy levels of some heavy ions and atoms (14-17). A Hartree-Fock-Pauli approximation was used extensively (27-31). Semiempirical calculations were also used for an analysis of d-electron shells in highly ionized atoms (34,36) as well as to obtain f-values for Na- and Ne-like ions (18-21). Table 1 presents references with indications of relevant ions or isoelectronic sequences.

2. Experimental studies of energy structure are listed in Table 2. Spectra of higher ionization stages and of those with higher ionization energies and of those

with higher ionization energies were obtained in the low-inductance vacuum spark (40,41) and in the laser-produced plasma (22-26,33). Line classifications in spectra of ions having d-electrons in the outer electron shell were investigated with the use of high-resolution spectrographs (32,34-39,42). The problem of line classifications in spectra of nickel ions appears especially important for interpretation of EUV solar spectra, where about 50% of lines remain unidentified (35).

### B. Molecular Data

Only some selected references are given in this report.

Computational methods for vibrational spectra of polyatomic molecules are presented in a book (43).

Fine structures of electronic spectra of diatomic molecules were investigated experimentally. Molecules containing atoms with unfilled d- and f-shells were studied for classification of their lower electronic states. This work is performed using flash photolysis techniques (45-47), gas-discharge tubes (48), thermal sources (49), and laser excitation (44). Fluorescence and absorption spectra in processes of chemical radiative collisions (50-51). A list of the molecules is given in Table 3.

This report refers to the activity of several research groups, mainly in the USSR Academy of Sciences.

TABLE 1

#### THEORETICAL CALCULATIONS (SELECTED REFERENCES)

EL - Energy Levels, W - Wavelengths,  
TP - Transition Probabilities, Life-Times, f-values

Ions or isoelectronic sequences	References
Ca XV, Fe XXI (EL,TP)	2
He-, Li-like (TP)	3, 4, 8, 11-13
Be-like (W,TP)	5
Fe XIX, Ni XXI, Fe XXIV (W)	6
Li-, Be-, F-like (TP)	7
K-vacancies (TP)	9
Be-, N-, O-, F-like (TP)	10
Zr XIII, Mo XV (EL)	14
Na-like (EL)	15
Yb I (EL,TP)	17
Ne-, Na-like (TP)	18-21
C-like (EL)	27

Ne-like (EL,W)	28
Ar I, K I, K II, Ca I, Ca III, Xe I, (EL)	29
Cs II, Ba I, Ba III, La II, La III	
Ne I (EL)	30
C-, O-, Ne-like, K X (EL)	31

TABLE 2

## LINE CLASSIFICATIONS AND ATOMIC ENERGY LEVELS

Ions, isoelectronic sequences	References
Mg IX, Zn XXVII	23
Mg XII - K XVIII (He-like)	24
Fe XVIII - Zn XXII, (F-like)	25
Ge XXIV, Se XXVI	
Ni XX, Cu XXI	26
Mn V	32
Cu XIX - Br XXV (Na-like)	33
Ge VI	34
Ni IX - Ni XII	35
Mn VII - Cu XI (K-like)	36
Y XIV - Mo XVII (Fe-like)	37
Ge VII	38
Sr XIII - Mo XVII (Fe-like)	39
Zr XXXI - Mo XVII (Fe-like)	
Zr XXXII - Mo XXXIV (F-like)	40
Zr XXXIII - Mo XXXV (O-like)	
Ag XXXVIII - Sn XLI (Ne-like)	41
Co VII	42

TABLE 3

## MOLECULAR SPECTRA

Molecules	References
Cs <sub>2</sub>	44
Mo <sub>2</sub>	45
Metal Hexacarbonyls	46
WO	47
LaF <sup>+</sup>	48
NdO	49
XeF*	51

References

Abbreviations: OS - Optika y Spectroscopiya,  
 LFR - Lietuvos Fizikos Rinkinis (Vilnius)  
 MNRAS - Monthly Notices Roy. Astron. Soc.  
 JQRST - J. Quant. Spectrosc. Radiat. Transfer  
 ADNDT - Atomic Data and Nucl. Data Tables

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