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#### 14a. SOUS-COMMISSION DES TABLES D'INTENSITES

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#### REPORT ON TRANSITION PROBABILITIES

*Note.* General references will be found in the Bibliography, in the same order in which they are quoted in the text. References to special transition probabilities, however, are collected into a separate section.

Since the last meeting of the IAU, the interest in fundamental data on transition probabilities has considerably increased. On one hand it became clear that the determination of cosmical abundances, for which they are needed, is of the greatest importance for a study of stellar evolution. On the other hand the investigation of the atomic processes in the chromosphere, in nebulae, in interstellar space, where thermodynamic equilibrium does not exist, requires a detailed knowledge of the atomic interactions with radiation and with particles. This increased interest has not only stimulated to new experimental and theoretical research, but also to special symposia, survey papers and general projects.

At the end of our 1958 report, we mentioned already the excellent monograph by Kolesnikov and Leskov, with an extensive bibliography, in which a serious attempt was made to compile a general table of  $f$  values for atoms and diatomic molecules. Shortly afterwards, in March 1959, a conference on Measurement and Calculation of Oscillator Strengths was held at the Physics Research Institute of the Leningrad State University (Report published in the same year). A bibliographic survey on transition probabilities up to 1958 is found in Varsavsky's thesis.

A very ambitious and long range project has been recently announced by the Bureau of Standards, Washington D.C., including the study of atomic properties, the production and study of high temperature gases, the interpretation of astrophysical and geophysical observations. The first section of this programme includes 16 paragraphs, of which three refer to the determination of transition probabilities in the broadest sense, to excitation and ionisation cross-sections. This unified effort will undoubtedly be of the greatest use to astrophysics.

A comprehensive survey of modern research on transition probabilities has been given by R. H. Garstang and a more recent one by H. van Regemorter. The importance of continuous absorption in stellar atmospheres, due to atomic and molecular negative ions, is studied in a paper of Branscomb and Pagel.

A systematic comparison between theoretical and observed  $f$  values has been made by Allen for the elements Sc, Ti, V, Cr, Mn, Fe, Co, Ni, reduced as well as possible to an absolute scale. The theoretical values were obtained simply from the sum rule or from Bates and Damgaard's formulae; the measured values were collected from the most reliable sources. For transitions which involve non-equivalent electrons only, all measured values are within a factor of three of the calculated scale. If equivalent electrons are involved and the upper EP is less than 4 eV, the scatter is much larger.

A comparison between theory and observation was also made for the special case of Fe I by Melnikov, on the basis of his own arc measurements. The agreement is bad for high and closely spaced levels (EP = 6 eV). Moreover it became clear that often the normal coupling does not apply.

#### EXPERIMENTAL DETERMINATIONS

(a) *In absorption.* The Soviet physicists went on applying Rozhdestvensky's method of anomalous dispersion. By this method, the product  $Nf$  is determined and  $N$  is generally found from the vapour pressure curve. In cases where this curve is not well known, Ostrovsky and his collaborators started recently working at a pressure, sufficiently low to avoid collision damping, and measured the equivalent widths of the strong lines, which are proportional to  $(Nf\gamma)^{\frac{1}{2}}$ . From the combination of both determinations, the value of  $\gamma_{\text{rad}}$  and the corresponding  $f$  was derived for the resonance lines of Mg I, Ca I, Sr I, Ba I.

For most of the metals, investigated by King *et al.* in the electric furnace, there are now also anomalous dispersion measurements. The merits of both methods have been compared by Ostrovsky and Penkin (See: Co and V). By measuring the anomalous dispersion it is difficult to investigate the absorption of atomic levels above 1.5 eV; moreover one cannot well separate doublets, closer than 0.5 Å; on the other hand the product  $Nf$  may be measured within a range of  $10^5$ , considerably greater than with the absorption method; the influence of stray light and ghosts is avoided. In general the results of both methods are in excellent agreement except for some faint lines.

The atomic ray method, first used by Kopfermann and Wessel, has now been applied also by King and his collaborators and has given some very reliable absolute values (Cu, Fe, Mn).

Burch, Branscomb *et al.* have applied their 1954 beautiful method to the determination of the continuous absorption by  $\text{H}^-$ ,  $\text{O}^-$ ,  $\text{O}_2^-$ . The ions are extracted from the striated column of a discharge tube and irradiated by the powerful, concentrated beam of an arc lamp; the stream of ejected electrons is measured. The precision is sufficient to determine the wavelength dependence and to detect deviations from the theoretical values, for example in  $\text{H}^-$ .

(b) *In emission, in the electric arc, in flames, in discharge tubes.* Hefferlin compared the results of emission measurements in the iron arc to the very reliable absorption measurements in

King's electric furnace. He concludes that self-absorption is practically absent, if the lower term of the transition has an excitation potential of at least  $2.2 \text{ eV}$ . Similar results were reached by him and his collaborators for Ti. This work confirms again the well-established assumption of thermodynamical equilibrium in the arc.

Especially interesting are the high-temperature arcs, used at the Kiel Physical Institute (C I, N II, O II, Si, Cl). They are stabilized by injecting a whirling gas or in other ways. With a current of 60 – 500 amps they reach temperatures of  $10\,000^\circ - 20\,000^\circ$ . The observations are made either side-on or end-on. It is found, however, that a mixture of two gases cannot be used to compare their transition probabilities, because the proportion of the gases changes in the arc (example: N + He). When determining the transition probabilities for Si, Hey avoided this difficulty by first making absolute determinations for Cl (from HCl), then blowing  $\text{SiCl}_4$  into the arc and reducing the values of Si to those of Cl. Each line is studied in a temperature range in which its intensity reaches a maximum; the temperature itself is derived from the intensity of another spectral line, which in that same range increases rapidly with temperature.

More recently, it was found that equilibrium conditions in a plasma develop in a surprisingly short time, often in  $10^{-7}$  sec, and that even a spark may be considered as a succession of equilibrium plasmas at decreasing temperatures. This justifies the use of light sources with a very short duration. The shock tube technique has been applied by Weber to the study of H- and by Keck *et al.* to  $\text{O}_2$ . The method of exploding wires, by which temperatures up to  $70\,000^\circ$  may be reached, has perhaps not yet been sufficiently exploited. It may be asked, whether the discharge in the Zeta instrument could be used as a light source for the study of astrophysically interesting ions.

Promising is the discharge tube with a hollow cathode, filled with Ar and He. With this source Khokhlov obtained fine results for Pb, as well in emission as in absorption.

The investigation of molecules in flames has been carried out and exposed in a very methodical way by Carrington for OH.

The direct measurement of life-times by the method of delayed coincidences has been made now also by Osherovich and Savich for He. It has the advantage that  $f$  values may be determined without a measurement of the number of atoms involved. We call attention to the paper of Guiochon, Blamont, and Brossel (*J. Phys. Rad.* **18**, 99, 1957), warning that a determination of the life-time of a resonance level is very dangerous, because there is nearly always imprisoned resonance radiation and repeated excitation.

(c) '*Astrophysical*' transition probabilities. New efforts have been made in order to perfect this method. M. E. and A. A. Boyarchuk, using the best measurements on the spectra of 7 stars, have calculated transition probabilities for 1184 lines of 21 atoms and ions, mostly belonging to the Fe family. The results are somewhat less precise than those determined in the laboratory.

Melnikov made an interesting attempt in order to find in such a way  $f$  values for the quadrupole multiplets of [Fe II], which cannot be obtained in the laboratory. The results, derived from  $\eta$  Car and XX Oph are very encouraging.

Most interesting are also the observations of Stoffregen and Derblom, who found a mean time-lag of 110 seconds between the apparition of the  $^+N_2$  bands in auroras, and the rise of the red lines ( $^1D - ^3P$ ); the life-time of the  $^1D$  level, thus found, checks very well with the transition probability, calculated by Garstang. In this case we are apparently able to determine the life-time of an atomic level by an observation in the open air, without instruments, simply looking on our watch when the colour of the aurora changes!

(d) *Theoretical.* We first call the attention to the thesis of Varsavsky, which gives an introduction to the calculation of transition probabilities in general, and then develops the 'Nuclear Expansion Method', based on the expansions of  $E$  and  $\Psi$  as introduced by Layzer. In its simplest form it was applied by the author to all atomic transitions, available in the literature, even to very complicated atoms. The results are accurate for  $\Delta n = 0$ ; for  $\Delta n = 1$  the results are often considerably in error; for  $\Delta n < 1$  the discrepancies seem to become smaller. It is possible to improve the method.

The study of multiplets, super-multiplets, and arrays has always played a large part in the determination of  $f$  values. Rohrlich, then Kelly and Armstrong completed and supplemented the tables of Goldberg and Menzel. The first author, making use of the Racah coefficients, derived general formulae for all multiplet strengths of astrophysical interest and obtained various sum rules, many of which are new. Dalgarno and Kingston even modified the theoretical  $f$  values for the metastable He levels so as to satisfy the sum rules. On the other hand Bersuker showed that departures from the sum rule occur; already long ago Fock has explained such cases by the effect of the inner-electron core which perturbs the outer levels.

Grant discussed the determination of monochromatic Gaunt factors for the free-free transitions of an electron of given velocity in the field of a positive ion. Tables are presented which make this calculation very quick; by a simple procedure it is possible to average over a Maxwellian velocity distribution.

The beautiful method of Bates and Damgaard, so useful for atomic lines and already extended to molecular bands, was applied by Burgess and Seaton to the calculation of continuous absorption coefficients.

Seaton gave a general theory of the Quantum Defect Method and Burgess and Seaton applied this to the calculation of transition probabilities for bound-bound and bound-free transitions. The results are consistent with those of Bates and Damgaard but may be used for larger values of the effective quantum numbers.

Vainstein also applied the method of Bates and Damgaard, but he represented the field of the inner atom by linearly deformed wave functions (see Ca, Cd, Cs etc.).

Ortenberg, calculating transition probabilities for molecules, applied (a) the method of Bates and Damgaard, (b) the Morse 'simplified' potential method. Differences of the order of 10% were found.

The Hartree-Fock method was still extensively used. Knox calculated transition probabilities for Ar, using (a) the wave functions alone, (b) the empirical energy parameters; differences of the order of 10% were found. Trefftz and her collaborators, working on He, took into account the non-orthogonality of the  $1S$  wave function and introduced a correlation factor of the Hylleraas type.

Geltman investigated in general the absorption by negative molecule ions near the threshold, and showed that they behave differently according to whether the molecule is homo- or hetero-nuclear and to the symmetry of the outer orbital.

Garstang completed his basic theoretical work on electric quadrupole transitions in Russell-Saunders coupling. For many astrophysical applications it will now be necessary to proceed towards more detailed calculations for intermediary coupling.

It does not seem that electronic machines have been used extensively for the calculation of transition probabilities. Vainstein emphasized and used this possibility.

A few special results concerning theoretical  $f$  values may be quoted. The absorption of the

H-ion has been the subject of many new calculations. Mitchell interpolated Chandrasekhar's tables for  $T$  and  $\lambda$ . Chandrasekhar revised his earlier calculations and used improved wave-functions for the ground state; then Chandrasekhar and Elbert improved again their calculation, by replacing the plane wave approximation for the free electron by the Hartree approximation. Both modifications resulted in minor changes only. Much more important, however, was the introduction of the effects of electron exchange and polarization, based on the calculations of Bransden *et alia*; the absorption coefficients, thus calculated by John for bound-free transitions, are the best thus far obtained. For the free-free transitions, the results of T. and H. Ohmura are in the infra-red 40–50% less than the earlier ones; they now agree better with the 'observed' solar values.

Special attention is drawn to the paper of Boggess, who calculated the emission, originating when a hydrogen atom and a hydrogen ion associate and form a hydrogen molecular ion  $H_2^+$ . The emission in the visible is about equal to that of  $H^-$ , but dominates in the ultra-violet at high temperatures; however it is still insufficient to account for the radiation of the nebulae, observed near 1300 Å. A related investigation was carried out by Erkovich, for the collision between two neutral H atoms, resulting in the formation of an excited molecule  $H_2$ ; also in this case the emission is of the same order as that of  $H^-$  in the visible, but dominates rapidly in the ultra-violet.

(e) *Forbidden lines.* Garstang completed his papers on the calculation of line strengths for forbidden transitions of astrophysical interest (*Proc. Camb. phil. Soc.* **54**, 383, 1958). He applied his methods to [Ni II], [Ni III], [Ne IV] and [Fe IV]. In the last case no spectral lines have been identified with certainty and the energy levels had to be theoretically estimated; transitions between the levels of a  $d^8$  configuration had not been studied before. Calculations by the same author for [Fe II] are in press.

Melnikov's derivation of [Fe II] transition probabilities by observation of stellar spectra has been mentioned under section (c).

#### HYPERFINE STRUCTURE

For the bibliography on this subject, up to 1959 we refer to the recent survey article by Kusch and Hughes in Flüggé's *Handbuch der Physik* **37/1**: 'Nuclear Spins and hyperfine structure intervals' (p. 100); a chronological list is found on p. 155.

We only draw the attention to recent work on the most important two elements:

$H^1$ ,  $H^2$ ,  $H^3$  Anderson, Pipkin, and Baird, *Phys. Rev. Letters* **4**, 69, 1960.

$He^3$  Brochard, Chantrel and Jacquinet, *J. Phys. Rad.* **19**, 515, 1958.

$He^3$  and  $He^4$  Chantrel, *Ann. Phys. (Paris)* **4**, 965, 1959.

#### COLLISIONAL EXCITATION AND IONIZATION OF ATOMS BY ELECTRONS

For all calculations about deviations from thermo-dynamic equilibrium, data on the collisional excitation and ionization of atoms by electrons are just as important as transition probabilities. To collect these physical constants seemed therefore a duty of Sub-commission 14a. This first attempt will be only provisional but may be improved in future.

Only the papers from 1957 on will be reviewed.

For the older literature, we refer to the following standard handbooks: Massey and Burhop, *Electronic and Ionic Impact Phenomena* (Oxford, 1952).

Massey, *Theory of Atomic Collisions*.

Massey, *Excitation and Ionization of Atoms by Electron Impact*.

(The last two chapters are part of Flügge's *Handbuch der Physik*, 36, 1956.)

We consider the inelastic collisions of electrons with atoms. The primary needs of astrophysics are concerned with the *total cross-section* (*c.-s.*) for excitation or ionization, while we are less interested in the *differential cross-section*, specified with regard to the angle over which the electrons are scattered. The cross-sections strongly depend on the velocity of the colliding electrons and are in general given as functions of the electron energy. A great part of the experiments and of the theories refer to high-energy electrons, for which the phenomena can be described in the simplest way. However for most astrophysical problems the collisions with slow electrons are more important.

The main results on cross-sections obtained up to 1956 may be roughly summarized as follows.

*Experimental:*

Ionization of He, Ne, Ar, Hg.

Excitation of H, He, Ne, Ar, Hg, Na, Ag, Zn, Cd, Tl, Pb; special attention has been given to the excitation of metastable levels of H, He, Ne.

*Theoretical:*

For high velocity electrons, the Born approximation gives good results: H, He, Ne, Hg, Na, Fe xiv; general formulae for complex atoms have been derived.

For slow electrons (energy  $< 7$  times threshold energy), the Born approximation underestimates the *c.-s.*, but in general it is not more in error than by a factor of 2. A more precise method is the E.D.W. method ('Exchange Distorted Wave'), on the condition that the exchange effects be fully accounted for; it was applied to H, He, He<sup>+</sup>, O, O<sup>+</sup>, O<sup>++</sup>, Fe xiv. Often more reliable is the 'Exact Resonance Approximation', which was applied to the  $p^2$ ,  $p^3$ ,  $p^4$  configurations of N I, II; O I, II, III; F II, III, IV; Ne III, IV, V; Na IV, V; Mg V; S II. By this last method, also the transitions between sublevels of the  $^3p$  ground term have been studied for O III and C II; moreover the excitation of allowed states in H I, O I, and Na I has been calculated.

The recent experimental work shows more and more details in the emission curve of a spectral line as a function of the electron energy; especially near threshold several subsidiary peaks appear, which are due to the contributions of the successively excited levels (this among others applies to He). By taking into account the optical transition probabilities, the direct excitation cross-section of a level may be determined. Phelps, again for He, has emphasized the danger of imprisoned resonance radiation and has made plausible, that some *c.-s.* values quoted in the literature are too great by a factor of 10.

As to the recent theoretical work, we call the attention to the general paper of Milford, by which it is possible in a few minutes to estimate the Born *c.-s.* for any atom and for any electron velocity. In order to reach more precision, lengthy calculations are in general necessary. Even for hydrogen, the excitation of the high levels can be computed only with effort; Boyd showed, how in such cases an interpolation method helps and how the introduction of differential ionization may be used for the highest terms. Numerical methods are often more precise than the classical approximations, especially near the threshold of excitation (See Marriott for H). Quite generally the computation of cross-sections may be considerably accelerated by electronic computers (See for example Ochkur for H, Vainstein for He).

The reporter is most grateful to the members of the Sub-Commission and to other scientists, who contributed to this report. Special thanks are due to Mrs Mitrofanova, who sent a very valuable list of Soviet publications.

M. G. J. MINNAERT  
President of the Sub-Commission

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*Special transition probabilities*

$T$  = theory;  $E$  = emission;  $A$  = absorption;  $D$  = anomalous dispersion;  $V$  = atomic ray;  $S$  = shock tube;  $C$  = coincidences;  $a$  = absolute values;  $r$  = relative values. If the author himself determined relative values but reduced them to absolute values by comparison with earlier results of others, we kept the character  $r$ .

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#### *Cross-Sections for Excitation and Ionization by Electrons*

The levels involved are indicated by their symbols;  $1^1S - n^1P$  means, that the  $1^1S$  atoms have been excited to  $2^1P$ , or to  $3^1P$ , or to  $4^1P$ , etc.;  $1^1S - \infty$  means ionization;  $1^1S - 2S$  means that  $1^1S - 2^1S$  and  $1^1S - 2^3S$  have both been studied.

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#### 14b. SOUS-COMMISSION DES SPECTRES MOLECULAIRES D'INTERET ASTRONOMIQUE

PRÉSIDENT: Professeur P. Swings, Directeur de l'Institut d'Astrophysique de l'Université de Liège, Cointe-Sclessin, Liège, Belgium.

MEMBRES: Herzberg, Junkes, McKellar†, Mme Moore-Sitterly, Nevin, Phillips.

EN PIEUX HOMMAGE À LA MÉMOIRE DE FRANCIS A. JENKINS  
ET ANDREW MCKELLAR

Les besoins des astro-spectroscopistes en informations sur les spectres de bandes ont certes continué à se manifester dans le domaine spectral usuel d'observation, approximativement de  $\lambda$  3000 à  $\lambda$  9000 Å. Mais il faut, à présent, penser aussi aux besoins en spectres moléculaires dans le domaine astronomique ultra-violet lointain qui commence à s'ouvrir à nous grâce aux observations à bord des fusées et satellites. On ne peut, non plus, négliger le domaine astronomique infra-rouge qui commence à être accessible, avec une résolution assez élevée, soit grâce aux nouvelles émulsions photographiques, soit par l'emploi des récepteurs infra-rouges de plus en plus sensibles, combinés aux systèmes dispersifs de principe nouveau récemment développés (par exemple l'interféromètre de Michelson avec transformée de Fourier). Dans l'infra-rouge astronomique, les spectres moléculaires joueront sûrement un rôle considérable.

Le spectre ultra-violet lointain de H<sub>2</sub> qui, jusqu'ici, n'avait pas présenté un intérêt astronomique très marqué, revêtira vraisemblablement bientôt une importance considérable, car H<sub>2</sub> est, sans doute, la molécule la plus abondante dans l'atmosphère de nombreux astres et, peut-être aussi, dans l'espace interstellaire et interplanétaire. Il est donc heureux qu'une nouvelle étude soignée du spectre de H<sub>2</sub> soit actuellement en cours (1) (2) (3) (4).