

COMMISSION 14: ATOMIC AND MOLECULAR DATA

DONNÉES ATOMIQUES ET MOLÉCULAIRES

Report of Meetings 21 and 26 November 1985

PRESIDENT: A. H. Gabriel

SECRETARY: W. L. Wiese

Business Session, 21 November 1985

1. Subject Matter of the Commission

A useful discussion was held on this topic following the debate which started at the Patras meeting. The principal question concerns whether the Commission should broaden its area to include the provision to astronomers of data in fields other than atomic and molecular physics, such as elementary particles, thermonuclear reactions, etc. Dr. A. H. Gabriel and a small committee had been charged with a task at Patras of reviewing this question. He reported the outcome of various consultations which resulted in the following conclusions and recommendations:-

a) The expansion to include these view fields of interest would lead to a substantial increase in the scale of the total activity and would result in a large diverse Commission, having few common interests.

b) Only certain sub-disciplines are suited to a critical compilation of data aimed at providing a service to astronomers. These generally have already a specialized medium available for dissemination. In other areas, the Commission works best when in a collaborative science role, in which each side participates a little in the other's scientific activity.

c) There is no evidence of pressure from the astronomy community for the Commission to move into these new areas.

d) Until or unless such pressure is evident, the Commission should continue to concentrate on the field of atomic and molecular data.

Following a discussion of this recommendation it was decided that for the present time the Commission should limit its field to atomic and molecular physics.

There followed a critical examination of the Working Group structure which resulted in the following changes.

Working Group 1 formerly included two district areas. The first concerns the primary standard of wavelength. It was felt that this problem had now moved into the field of metrology and was not of sufficient concern to astronomers. It should be dropped from the Commission's work. The remaining area concerns wavelength standards for practical spectroscopy. This should be incorporated in the Working Group which deals with Atomic spectra.

Working Group 3 formerly concerned collision cross-sections and line broadening. This wide topic had always been split in two for preparing the Report, and it was agreed that it should now be dealt with by two Working Groups. The name of the first should be modified to Collision Processes in order to cover rate coefficients, etc.

Working Group 5 on Molecular Spectra should be expanded to include other molecular data, such as transition probabilities and dipole moments but not collision data. Its name should be changed to Molecular Structure and Transition Data.

A discussion was held on the manner in which the Commission carries out its work. There was strong support for a collaborative mode. It was felt that at the General Assembly meeting, joint commission meetings were most valuable and should be encouraged, with the astronomers taking a lead in formulating the programme.

2. Appointment of offices for the period 1985-8

The following committee was approved:-

President: R.W. Nicholls
Vice President: S. Sahal
Organizing Committee:
A. H. Gabriel
T. Kato
F. J. Lovas
S. L. Mandelstam
H. Nussbaumer
W. H. Parkinson
Z. B. Rudzikas
W. L. Wiese

Following the earlier discussion on reorganisation, the Working Groups and their Chairmen were approved as follows:-

1. Atomic Spectra and Wavelength Standards (excluding primary standards),
W. C. Martin
2. Atomic Transition Probabilities, W. L. Wiese
3. Collision Processes, A. Dalgarno
4. Line Broadening, (A. H. Gabriel to discuss possible Chairman)
5. Molecular Structure and Transition Data (R. W. Nicholls to recommend
Chairman)

The Commission approved the acceptance of 11 names from list A as new members of the Commission

Scientific Session, 26 November 1985

1. Photo Rate Coefficient

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The original list of species for which we calculated photo rate coefficients for dissociation, ionization, and dissociative ionization was limited to those of

interest in comet coma studies. This list has now been expanded to include species of interest to planetary atmospheres, pollutants in the earth atmosphere, and interstellar clouds. Rate coefficients are defined by

$$k \equiv \int_0^{\lambda_{th}} \tau(\lambda) e^{-\tau(\lambda)} F(\lambda) d\lambda,$$

where $\tau(\lambda)$ is the cross-section for the appropriate process taking into account the branching ratio, $\tau(\lambda)$ is the optical depth as measured from the top of the atmosphere or interstellar cloud, $F(\lambda)$ is the photon number flux, and λ_{th} is the wavelength at threshold. We also calculate the mean excess energy of the photolysis products

$$E_X \equiv ch \int_0^{\lambda_{th}} \left(\frac{1}{\lambda} - \frac{1}{\lambda_{th}} \right) \tau(\lambda) e^{-\tau(\lambda)} F(\lambda) d\lambda / k.$$

We use detailed, wavelength dependent cross-sections for all process for which such data are available, including predissociation and autoionization. But since the measured solar (or interstellar) flux is only available for finite wavelength bins, the above integrals are replaced by summations of the appropriate values in these bins.

Rate coefficients and mean excess energies have been calculated for about 90 atomic and molecular species using a detailed unattenuated ($\tau = 0$) solar spectrum for the quiet sun at 1 AU heliocentric distance. Similar calculations are being done for the active sun and for the interstellar radiation field. Several more atomic and molecular species will be added.

Cross-sections averaged over larger wavelength bins will be made available on magnetic tape so that users can calculate effective photo rate coefficients with suitable optical depth effects. These data will be too crude if Doppler shifted coincidences of atomic or molecular spectral lines with solar spectral features are important in the determination of the rate coefficients.

IMPROVEMENTS IN ATOMIC TRANSITION PROBABILITY DATA

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Atomic transition probability data for many atomic spectra have been improved recently, especially for the ions and neutral atoms of lighter elements. The overall distribution of new literature papers containing numerical data for the three-year period 1982-1984 is presented in Figure 1.

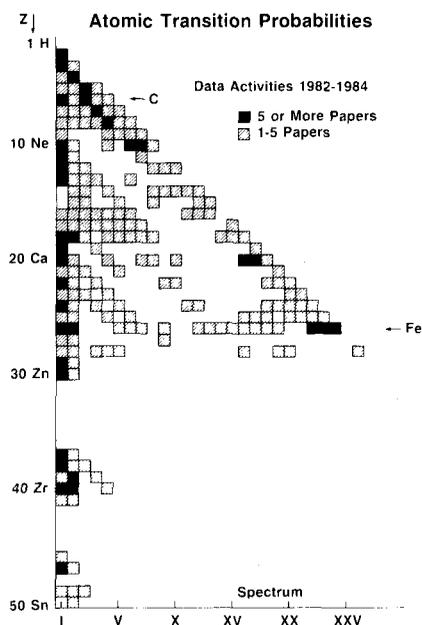


Fig. 1. Distribution of literature references on atomic transition probabilities for the time period 1982 to 1984.

This overview shows clearly that a large part of the new work is concentrated on neutral and singly ionized species. Furthermore, among the more highly ionized atoms, recent data determinations have concentrated primarily on ions of the helium-, lithium-, and beryllium-like isoelectronic sequences, which are represented by the longest diagonal lines in the figure.

From a detailed study of the literature, four major conclusions emerge:

(1) For neutral atoms of nuclear charges Z smaller than 20, atomic structure theory has advanced to a stage where it is capable of delivering quite accurate data. An important atomic structure problem is the mutual interaction between the atomic electrons, leading to the electron-correlation problem. Thus, atomic eigenstates are best described in terms of combinations of configuration state functions, each of which is a product of single-electron functions (orbitals). Such multi-configuration or superposition-of-configuration treatments, carried out within the self-consistent field or Hartree-Fock model, are the most powerful theoretical approaches which show in many cases excellent agreement with accurate experimental data, typically at the 10% level.

(2) Turning to elements of the iron group ($Z = 21-28$) with their increasingly complex valence shells, one observes that theoretical methods are still inadequate for the accurate determination of atomic transition probabilities while experimental approaches have made significant progress. Thus measurements are the major source of accurate data and numerous accurate results have become available on both neutral atoms and singly ionized ions in recent years. A very productive and successful approach is to combine two quite different experimental techniques:

- (a) Determinations of atomic lifetimes for those levels which interact directly with the ground state via electric dipole transitions (resonance transitions).
- (b) Relative emission (or absorption) measurements, including "branching ratio" measurements, for all transitions from (or to) such upper levels, as well as neighbouring levels.

Thus the strengths of the lifetime technique and emission or absorption methods are combined, i.e., the lifetime determinations yield accurate absolute scales for the relative emission or absorption line strengths covering the individual lines involved with each level. The resulting data are estimated to be quite accurate, typically in the 10-25% accuracy range, because atomic level lifetimes can be reliably determined with delayed coincidence methods using selective tunable laser excitation; furthermore, the emission or absorption measurements, being restricted to relative measurements from or to the same atomic level are independent of the properties of the source and no diagnostic measurements have to be made. When the measurements are extended to neighbouring levels, some source properties must be known, but they do not enter sensitively into the results. With the combination of these two techniques, data for the spectra of neutral and singly ionized iron, cobalt, and nickel have been drastically improved in recent years.

(3) For the heavier elements beyond the iron group many recent experiments have been concerned with the determination of atomic lifetimes. This is due to the advent of the above-cited laser excitation technique which allows a wide range of atomic species to be studied. These lifetime determinations yield the transition probabilities of a few resonance lines but do not provide a comprehensive description of the spectrum. Emission, absorption or anomalous dispersion methods involving many transitions similar to the above-described case for the iron group elements are necessary to complete the task.

(4) For highly stripped ions, only a few electrons remain and the situation for theoretical work becomes similar to that of light neutral atoms (case (1)). However, an important difference is that the nuclear charge is strongly increased, and thus relativistic effects will become noticeable. Thus relativistic multi-configuration techniques have been developed and applied to many light-element isoelectronic sequences. For highly stripped ions of Fe-group and heavier elements, relativistic effects become increasingly important.

This brief summary thus shows that newly developed theoretical and experimental techniques as well as the combination of the strong features of such techniques have brought about significant improvements in atomic transition probability data.

Reference

1. W. L. Wiese, in "Reports on Astronomy 1985," Comm. 14, D. Reidel Publ. Co., Dordrecht, Holland.