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COMMISSION 14: ATOMIC AND MOLECULAR DATA[1]

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In recognition of its special interdisciplinary character, IAU Commission 14 is linked directly to the Executive Committee. The Commission's role is to inform the astronomical community of new developments in the diverse fields of research which involve atoms and molecules. Conversely it endeavours to sensitize the research community active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commision 14 tries to foster long term relations and collaborations between the two communities and, when necessary, to alert funding authorities to the specific needs of ground and space based astronomy for specific atomic and molecular data.

This report is one of the main contributions of Commission 14 to the information of the astronomical community. Several meetings concerned, at least in part, with the need and availability of atomic and molecular data for astrophysics were also sponsored or co-sponsored. In the last triennium, Commission 14 cosponsored IAU Symposium 194 "Astrochemistry: From Molecular Cloud to Planetary Systems" held in Sogwipo (Korea) from Aug. 23 to 27, 1999 and organized by Commission 34. A Joint Discussion: JD1 on "Atomic and Molecular Data for Astrophysics, New Developments, Case Studies and Future Needs" has been planned for the XXIVth IAU General Assembly in Manchester (Aug. 7-19, 2000) and cosponsored by Commissions 15, 16, 29, 34, 36, 40 and 44. Several other Joint Discussions to be held at the Manchester General Assembly are co-sponsored by this commission.

The present report comprises six sections established by the specialized Working Groups of Commission 14. It is made available on the Commission 14 Website:
`http://ww.obspm.fr/IAU14`
and its mirror `http://cfa-www.harvard.edu/amp/iau14`.

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[1]Committee of the Executive Committee.

4. WORKING GROUP 4: LINE BROADENING

PRESIDENT: C. STEHLE
VICE-PRESIDENT: G. PEACH

The field of line broadening has been very active during the last three years, as indicated by the proceedings of the 14th International Conference on Spectral Line Shapes (ICSLS), which was held in State College (Pennsylvania, USA) in 1998 (Herman 1999) and by the Supplement 5 to the Bibliography on Atomic Line Shapes and Shifts for the period April 1992 to December 1997 (Lesage & Fuhr, 1998). This bibliography is also available at the following World-Wide Web addresses:

`http://www.mesunb.obspm.fr/travaux/SRPR1F.html`

`http://physlab.nist.gov/PhysRefData/Linebr/html/reffrm0.html`

An Atomic, Molecular & Optical Physics Handbook was published in 1996 (Drake 1996), and it contains two chapters (19 and 57) relevant to spectral line broadening problems. The first one, written by A. Gallagher, is devoted to the neutral line shapes and radiation trapping. The second, by G. Peach, summarizes helpful basic theoretical expressions, commonly used in line shapes theory.

We shall restrict our report to theoretical and experimental work that may be of interest for astrophysics, with special attention to convenience and reliability.

4.1. Stark Broadening

In the field of Stark broadening, the recent book, "Principles of Plasma Spectroscopy", by Griem (1997), gives a helpful, updated compilation of the two older ones by the same author (Griem 1964, 1974). The first section deals with the Stark broadening of isolated lines which may be described using a collisional approach. The lines of hydrogen, hydrogenic ions and helium are discussed separately; these lines, which are sensitive to many-body effects, require specific treatments.

Isolated Lines The semi-classical formalism provides a powerful tool for the rapid calculation of line widths and shifts with a mean accuracy of $\pm 30\%$. As a consequence, the number of transitions considered has increased rapidly. In this period for example, data for lines of C V, P IV, P V, Be III, B III, S V, Ca IX, Ca X, Si XI, Si XIII, Na X, O VII, Mg XI, Sc X, Sc XI, Ti XI, Ti XII, K VIII,K IX (Dimitrijević & Sahal-Bréchot 1-10) Mn II, Mn III, Ga III, Ge III, Ge IV (Popović & Dimitrijević 1998), Xe II (Popović & Dimitrijević 1996), Ba I, Ba II(Dimitrijević & Sahal-Bréchot 1996b), Sr I (Dimitrijevic & Sahal-Bréchot 1997), Mg I (Dimitrijevic & Sahal-Bréchot 1996a) and OI (Ben Nessib & Ben Lakhdar, 1996), have been computed. Despite the large number of tabulated results, accessible by internet at the Centre de Données de Strasbourg:

`http://cdsweb.u-strasbg.fr/Abstract.html`.

The audience of these results could be greatly enlarged if the data was also presented in the form of a data base. Alternatively, the semiempirical formulas (Dimitrijević and Konjević 1980) also give rapid results, but they are somewhat less accurate.

One notes also the large number of experimental determinations of line widths and/or shifts for the transitions: NII, NIII and NIV ($3s-3p$ and $3p-3d$, Milosavljević and Djenize 1998), NII (463.054 nm, Djenize and Milosavljević, 1998), Ne I ($3p-3s, 3p-3d$, Del Val et al. 1999), B III ($2s-2p$, Griem et al. 1997), Na I (467-498 nm, Kettlitz and Oltmanns 1996), Si I (220, 250, 288 nm, Srecković et al. 1998), Si II (386, 385 nm, Wollschlager et al. 1997), C II, N II, O II, F II and Ne II ($3s-3p$ and $3p-3p$, Blagojević et al. 1999a) Xe III ($4f-6d, 5d-4f, 5d-6p, 6p-7s, 6s-4f$, Romeo y Bidegain et al. 1998), O II ($3s-3p, 3s'-3p', 3p-3d, 3p-4s$, Djenize et al. 1998), Ar I (425 nm, Djurović et al. 1997), Ar II (90 spectral lines, Pellerin et al. 1997), and the study of the variation of the widths/shifts along the Be-sequence ($3s-3p$, Wrubel et al. 1998), the Li- and Be- sequences

(C IV, N V, O VI $3s^2S - 3p^2P$, and B II, C III, N IV, O V $3s^3S - 3p^3P$, Blagojević et al. 1999b), the B-like sequence (N III, O IV, F V, $3s - 3p$ and $3p - 3d$, Blagojević et al. 1996).

Hydrogen Lines In the case of the lines of hydrogen, extensive calculations have been carried out. For example, the tabulation of the Paschen lines, using the Model Microfield Method, give both the line centres and the line wings to an accuracy better than 15% (Stehlé 1996a). Also, precise Monte Carlo calculations of the line width of the Paschen α line have been made by Cardenoso et al. (1997), and this method is designed for intermediate and high density plasmas. Accurate full-profile computations have been performed for the Paschen α, β and Brackett α lines (Motapon et al. 1997) and the Lyman α line (Motapon 1998), using a quantum description of the collisions with ions and electrons. In the line centre, this description is limited to low-density plasmas.

At low density, the line shapes of hydrogen have a Lorentzian shape. An analytical expression for their width is given by Stehlé (1996b), together with parameters necessary for the computation of the Holtsmark intensity in the line wings.

The far wings of the hydrogen lines exhibit molecular satellite features which, in astrophysical plasmas, are attributed to the transient formation of H-H or H-H^+ molecules. These satellites are used to determine the gravity in DA white dwarfs. Recent progress has been made by including the variation of the radiative dipole moment during the collision for the Lyman β line (H-H^+ satellites, Allard et al. 1998a) and for the Lyman α line (H-H, and H-H^+ satellites, Allard et al. 1998b).

Two new theoretical research areas have been developed. The first concerns the study of the lines of hydrogen in the presence of magnetic fields (Günter and Könies 1999, Brillant et al. 1998). These developments may be useful in the future for the characterization of magnetic stars. The second is the study of the shift and asymmetry of the Balmer α, β and γ lines; these effects are produced by short-range interactions with the plasma charges (Günter and Könies 1997).

Helium Lines The study of the intensity and shape of forbidden transitions in helium stopped in 1975, probably because of its intrinsic difficulty. The subject has recently been revisited by Beauchamp et al. (1997), for application to Helium rich (DB) White Dwarfs, using a static approximation for the interaction between helium and the plasma ions. They calculated the line shapes for the $2p - ns$, $2s - np$ and $2p - nd$ transitions which are in the optical range. The Stark widths and shifts of allowed infrared helium lines (3p-7d, 3d-7f, 3p-9d, 3d-12f, 3p-10d) have also recently been studied theoretically by Terzi et al. (1998), in the semi-classical approximation, both in the impact and quasistatic limits.

Lines of H-like Ions The study of lines of hydrogenic heavy ions is only important in opacity calculations for stellar interiors, or for the evaluation of the radiative forces in stellar envelopes. This requires the description of the full line, from the centre to the line wings. One may use the recent parametrization given for the lines of C, N and O by Gonzalez et al. (1998).

4.2. Line Broadening by Foreign Gases and Molecular Line Broadening

Introduction and Reviews During the period 1996-9, there has again been considerable activity in the field of spectral line broadening by neutral species, both theoretically and experimentally, and much of the work has been stimulated by the need to interpret observations of the atmospheres of planets and cool stars. The proceedings of the 14th International Conference on Spectral Line Shapes (Herman 1999) include a special section on astrophysical and atmospheric applications. Valuable databases that provide information on many molecular species for spectroscopic studies of atmospheres have been further extended, see the reviews of Wenger & Champion (1998), Rothman et al. (1998) and Jacquinet-Husson et al. (1999). Szudy & Baylis (1996) have reviewed Unified Franck-Condon theory and its

applications to the far wings of pressure-broadened profiles, rainbow satellites and the collisional redistribution of radiation. Gamache et al. (1998) have presented a critical review of data for the pressure broadening and shift of spectral lines of ozone.

It is not the aim of this report to be exhaustive; the papers cited have been chosen on the basis of their potential astrophysical interest. The preceding reviews contain many references, and so only papers not included in them are listed below.

Broadening of Atomic Lines Results have been obtained for the broadening of far-wing profiles of lithium lines by helium (Behmenburg et al. 1996), and general tables for calculation of the broadening of atomic p–d, d–p, d–f, and f–d transitions by neutral hydrogen are presented by Barklem & O'Mara (1997, 1998) and Barklem et al. 1998). Results for the broadening of Na D lines by O_2, N_2, CO_2 and H_2O and Mg and Ca lines by N_2 are given by Nefedov et al. (1999) and El Ghazaly et al. (1999).

Broadening of Molecular Lines In addition to the research described in the reviews of Wenger & Champion (1998), Rothman et al. (1998) and Jacquinet-Husson et al. (1999), the pressure broadening and shift of various molecular bands has been investigated either experimentally or theoretically and the molecules are listed below together with their perturbing atomic or molecular species. They are: H_2–He, H_2 (Michaut et al. 1998, Joubert et al. 1999), $^{12}CH_3D$–He, H_2, N_2 (Boussin et al. 1999), H_2S–He, H_2, N_2, O_2 (Flatin et al. 1999, Ball et al. 1999), CO–He, Ar (Sinclair et al. 1998), CO_2–He, Ar, CO_2, N_2, O_2 (Rodrigues et al. 1998, Vigasin 1999, Ma et al. 1999, De Rosa et al. 1999), N_2–N_2 (Buldyreva et al. 1999), NH_3–H_2,NH_3 (Irwin et al. 1999, Birnbaum et al. 2000), N_2O–He, N_2 (Bouanich et al. 1998), $^{16}O_2$–$^{16}O_2$ (Schermaul & Learner 1999), $^{16}O^{18}O$–$^{16}O^{18}O$ (Schermaul 1999) and OH–He, H_2, N_2, O_2 (Park et al. 1999).

Collision Induced Spectra Collision-induced absorption in dense atmospheres of cool stars has been reviewed by Borysow and Jørgensen (1999). Recent publications include studies of far-infrared bands of H_2, CO_2, O_2 and liquid methane (Brodbeck et al. 1999, Gruszka & Borysow 1999, Moreau et al. 2000, Birnbaum et al. 1999), and of the fundamental band of CO broadened by N_2 (Luo et al. 1999).

Data Bases Currently available are the following databases:

Spherical Top data System (STDS), `http://www.u-bourgogne.fr/LPUB/sTDS.html` ,

High resolution Transmission (HITRAN-96), `http://www.hitran.com`,

and Gestion et Etude des Informations Spectroscopiques Atmosphériques (GEISA-97). (`http://www.ara.polytechnique.fr/alexei_ index.html`).

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