

WORKING GROUP 3: COLLISION CROSS SECTIONS AND LINE BROADENING**A. LINE BROADENING**

The proceedings of the 6th and 7th International Conference on Spectral Line Shapes shown the general state of advances of the subject. Though a great part of the actual content lies outside the present interest, a number of useful results for astrophysical purposes can be found therein and will be quoted hereafter.

1. Stark Broadening of Hydrogen or Hydrogenic Lines**1.1 HYDROGEN LINES AT MODERATE DENSITIES AND TEMPERATURES**

Hydrogen line profiles at low densities have been revisited. New calculations have been performed for H α at typical astrophysical densities (smaller than 10^{14} cm $^{-3}$), demonstrating the validity of the impact model in the center and the neighbouring wings for proton collisions and electrons as well: this has been done by comparing results obtained with model microfield method with standard impact (semi-classical perturbation method and quantum exact resonance method) theories. Analytical formulae have been given(4,5) and have been shown to be now in agreement(6) with available recent experiments (contrary to previous calculations based on impact electrons and quasistatic ions). On the other hand new measurements of the cores of H α and H β have been published(7,8) which are in agreement with other recent experiments(9).

The first calculations of hydrogen Stark broadening in the presence of a magnetic field have been obtained(10,11) by using unified classical straight path theory: case of Ly α , Ly β , H α for $N_e \sim 10^{15}$ cm $^{-3}$, $T = 5 \cdot 10^3$ to $2 \cdot 10^4$ K, $B = 2.5 \cdot 10^3$ to $4 \cdot 10^4$ Gauss and two orientations of the field (longitudinal and orthogonal). Since the influence of the strength and orientation of the field appears to be not negligible, the use of those results appears to be highly advisable for analysis of magnetic stellar atmospheres: Ion dynamic effects are shown to be relevant in the near wings whereas the ions can be considered as static in the far wings(12). Extensive tables are provided(13).

Plasma satellites in the presence of non resonant, coherent and polarized radiation(14) and in the presence of non coherent and unpolarized radiation field(15) have been investigated: the effect of radiation shifts the satellites and enhances their intensities. Observational evidence of that effect among chromospheric lines has been indicated(16).

1.2 HIGH TEMPERATURES AND DENSITIES AND HYDROGENIC LINES

A very important effort is actually directed toward very hot and dense plasmas, in view of controlled fusion studies. Inertially confined, laser-produced plasmas are concerned.

This effort should benefit to astrophysicists studying hot and dense stars. Theoreticians focus their attention on strong correlation effects. Due to the exceptionally intense electric and magnetic field of laser compressed plasmas, consequent perturbations of spectra occur (for $Z > 10$ a few bound states may remain) and the physics of the plasma itself is complicated by strong interactions among the constituent species and by near quantum degeneracy. These high density effects on atomic and ionic plasmas have been discussed(17). The electric microfield distribution is the object of various theoretical studies. Though quantum corrections to the electron screening of the ions have been shown to be weak (less than 10%) for actually laser produced plasmas(18), quantum microfield distributions studies seem to be relevant(1,19) in view of the future development of higher temperatures and densities: quantum effects of both diffraction and degeneracy appear when the electron gas Fermi temperature approaches the temperature of the system. Concerning classical electric microfield

distributions, the case of strongly coupled plasmas deserves attention: a new method based on the expression of the Fourier transform of the microfield distribution gives a good agreement with computer simulations(20). A critical comparison of several approximations has been provided(21), including actual versions of the nearest neighbour, next nearest neighbour approximations together with two approximations based on independent perturber models; comparisons with Monte Carlo simulation techniques have been made. The formal theory of line shifts due to quasistatic ions has been reconsidered, suggesting that a self-consistent treatment of plasma correlations requires a much more complete theory(22). In these plasmas, dynamic terms may be as important as static ones when second and higher order terms are taken into account for the calculations of line shifts in hydrogen(23). By using a systematic instead of a phenomenological justification for long range cutoffs and treatments of initial correlations, it has been confirmed for ionized emitters that the dominant collective effect of the long ranged electron-electron Coulomb interaction is to screen the binary radiator-electron collision(24). The plasma polarization shift has a region of interest, because it is expected to be large at high Z and high densities. In fact recent measurements(25) ($P\alpha$ of He II at $kT = 4$ eV and $N_e = 1.6 \cdot 10^{23} \text{ m}^{-3}$) seem to infer that the most probable cause of the shift is the electron impact effect, provided it is properly calculated by including plasma polarization, and that a quasistatic approximation cannot be used; on the other hand line profiles of $P\alpha$ and $P\beta$ of He II have been measured(26) ($N_e = 10^{23}$ to $5 \cdot 10^{23} \text{ m}^{-3}$ and $kT < 11$ eV) in a gas liner pinch: the results can be explained by a combination of the electron impact collisions and by the quadrupole quasistatic effect which should be responsible for the obtained asymmetry. Using a pulsed linear discharge, Stark profiles of Balmer α , Balmer β , and $P\alpha$ line of He II have been measured(27) at $kT = 3.8$ eV and $N_e = 5.5 \cdot 10^{22} \text{ m}^{-3}$: these results show the importance of ion dynamics effects and also of fine structure effects for Balmer α . Radiator ion motions and low frequency electron produced fields have been included in a standard theory using impact electrons and quasistatic ions(1) and the results fit more favourably the experiments than the MMM method: profiles of $Ly\alpha$ and $Ly\gamma$ of Ar^{17+} ($N_e = 5 \cdot 10^{23} \text{ cm}^{-3}$, $T = 4.6 \cdot 10^6$ K) have been calculated. On the other hand, $Ly\alpha$ and $Ly\beta$ of Ne^{9+} and Ar^{17+} profiles have been computed(28),(29) ($N_e = 2 \cdot 10^{23} - 10^{24} \text{ cm}^{-3}$, $T = 1.2 \cdot 10^6$ and $1.2 \cdot 10^7$ K) by means of a Baranger-Mozer quasistatic distribution revised and extended to dense and hot binary ionic mixtures: A synthetic spectrum model and fast codes have been developed(30), using standard theories (impact electrons and quasistatic ions): line shapes of the Lyman and helium series have thus been calculated for Al , Na , Si , Cl , Ar , Ca , Ti . Typical results have been drawn and the fitting method based on the comparison of the synthetic to the measured spectrum ($T_e = 750 \pm 100$ eV, $N_e = 2 \pm 0.3 \cdot 10^{21} \text{ cm}^{-3}$) seems to be accurate for determining temperature and densities. A new field of measurements has opened up with the advent of multi-beam lasers capable of compressing symmetrically spherical targets: densities as high as $1.5 \cdot 10^{24} \text{ cm}^{-3}$ and temperatures ~ 1 keV can be attained(31,32): line profiles of $Ly\alpha$, $Ly\beta$ of Ar^{17+} and lines of Ar^{16+} are reported.

2. Stark Broadening of Overlapping Lines of Helium

The basic ideas of the model microfield method (MMM) have been reviewed as well as various theoretical and experimental works devoted to ion dynamics effects of overlapping helium line profiles(33). Improved Stark profiles of the He I 4471 Å have been computed using the MMM at astrophysical densities(34). New experiments(35) concerning He I 4471 and 4922 Å have been made at $N_e = 10^{21}$ to $3 \cdot 10^{21} \text{ m}^{-3}$, $T = 2 \cdot 10^4$ to $3 \cdot 10^4$ K, extending existing measurements towards higher temperatures and densities: these results are rather well described by the MMM; ion dynamic effects considerably modify the line shape of the forbidden components. Simple empirical formulae useful for determination of electron densities of helium plasmas have been proposed from the interpretation of experiments(36): the only parameters which enter the formula leading to N_e are

TABLE I

Stark broadening and shift of isolated line: reference data
E = experimental, *T* = theory, *SC* = semi-classical, *SE* = semi-empirical,
MMM = model microfield method.

Lines	References and method	Range of plasmas parameters Ne cm ⁻³ , T ₀ K
Cl 2p3s-2p4p (1p ⁰ -1D, 1p ⁰ -1P, 1p ⁰ -1S, 3p ⁰ -3S, 3p ⁰ -3P)	(38), E(wall stabilized arc)	7.4-8.3 10 ¹⁶ , 11350, 12330
HeI 56 lines (UV, visible, IR)	(39), T (SC)	10 ¹⁶ , 2.5 10 ³ -8 10 ⁴
HeI 36 lines (4<nupper<10)	(40), T (SC)	10 ¹⁶ , 2.5 10 ³ -8 10 ⁴
HeI 42 lines (2<nupper<6)	(41), T (SC)	10 ¹⁶ , 510 ³ -410 ⁴
HeI 6678, 5876, 3889 Å	(42), E(laser)+T(MMM)	10 ¹⁷ -2 10 ¹⁸ , 2 10 ⁴
ArI 4s-4p array	(2), E(wall-stabilized arc)	10 ¹⁷ , 1.3 10 ⁴
ArI 4300 Å	(43), E(wall-stabilized arc)	1.1-11 10 ¹⁶ , 9 10 ³ -1.5 10 ⁴
XeI 6s-6p ¹ , 6s-7p	(44), E(Shock-tube)+T(SC in j-k coupling(45))	2.2-10 ¹⁶ , 9.2 10 ³ -1.25 10 ⁴
Heavy elements (BrI, CdI, CeI, HgI, PbI, RbI, SnI, ZnI)	(46), T (SC)	10 ¹⁶ , 5 10 ³ -4 10 ⁴
Heavy ionic solar lines (TII, MnII)	(47), T (SC, SE)	
F I	(48), E(wall-stabilized arc) + T (SC)	1.4 10 ¹⁷ , 1.4 10 ⁴
MgI 2852 Å, MgII 2795, 5, 2802.7 Å	(49), E(wall-stabilized arc)	1.1-1.6 10 ¹⁷ , 1.3-1.4 10 ⁴
CaII 3933.7, 3968.5 Å	(50), E(wall-stabilized arc)	10 ¹⁷ , 1.3 10 ⁴
KI ns-4p (n=7-10), nd-4p (n=5-8)	(51), E(wall-stabilized arc)	2.10 10 ¹⁵ , 2.9 10 ³

Lines	References and method	Range of plasmas parameters Ne cm ⁻³ , T _e K
SiIII 3p, 2D-4p 2P ⁰ , 4s 2S-4p 2P ⁰ , 3d 2D -4p 2F ⁰ 2P ⁰ -5s 2S, 4p 2P ⁰ -4d 2D	(52), E(Shock-tube)	0.3-1.4 10 ¹⁷ , 1.6-2-2, 10 ⁴
SiII, SiIII	(53), T (SE)	
Xe II 5339, 5372, 5419, 5439 Å (6s-6p, 6p-6d)	(54), E (Shock-tube)	0.1-1.5 10 ¹⁷ , 7.8-8.4 10 ³
XeII 6s-6p, 5d-6p	(55), (Shock-tube)	0.6-1.8 10 ¹⁷ , 1.0-1.2 10 ⁴ K
SII 5320, 5453, 4525 Å	(56), (wall-stabilized arc)	7 10 ¹⁶ , 1.2 10 ⁴
SIII, Ca III, S IV	(57)	
OIII, SiII; OII, Ca III, ArIV; FeII, ArII; OIII, SiII: several lines of homologous structure	(58), T (SE)	
CIV, 12 lines (985-5805 Å)	(26), E(gas liner pinch)	10 ¹⁷ -5 10 ¹⁷ , kT = 11 eV
CrII 4s 4D-4p 4F ⁰	(59), E(Shock-tube)	2.55 10 ¹⁷ , 1.8 10 ⁴
Be like ions	(60)	
TiII, MnII + others already available	(61), T (SE, SC)	10 ¹⁷ , 2.5 10 ³ -2 10 ⁴

the ratio of the forbidden peak to the allowed peak intensity, the ratio of the minimum intensity between the two lines to the allowed peak, and the forbidden to allowed peak separation $N_e = 10^{21}$ to $10^{22} \text{ m}^{-3} \pm 15\%$, $T_e = 10^4$ to $1.5 \cdot 10^4$.

3. Stark Broadening of Isolated Lines in Moderately Dense Plasmas

A critical review and a tabulation of selected data concerning experimental Stark widths and shifts has been carried out(37) for non hydrogenic spectral lines of ionized and neutral atoms: it concerns the period 1976-1982. A number of new data of astrophysical interest have been obtained and are collected in Table 1. Systematic trends of Stark broadening parameters as function of the principal quantum number have been studied(2),(39),(40),(52) and can be used for obtaining missing data, by interpolation or extrapolation (when possible). The increase of accuracy of the measurements permits now the determination of rather small features which were not attainable even in the recent past and thus broadening by ions becomes measurable: asymmetry patterns of Stark broadening of several CI lines have been measured ($N_e = 7.4 - 8.3 \cdot 10^{16} \text{ cm}^{-3}$, $T = 11350 - 12230 \text{ K}$), and are in qualitative agreement with the quasistatic theory of ion broadening due to the quadratic Stark effect; the same conclusion arises from(44). Measured Stark broadening parameters are in general satisfactory agreement with semi-classical impact calculations of MMM calculations when they exist. The use of j - l coupling instead of L-S coupling for the case of heavy atoms is responsible for great differences(44), especially when quadrupole effects are important. However, a number of experimental results still disagree with theoretical calculations and this remains to be explained; in(26) (case of C IV lines) the disagreement holds especially for lines originating from the first excited levels, for which quantum effects may be important. This has to be compared to the fact that the new experiments performed on the case of Mg II 2s-2p(49) and Ca II 4s-4p(50) agree now with quantum close coupling calculations, whereas they disagree with the semi-classical ones: this had been expected for a long time but had been contradicted by previous measurements.

4. Line Broadening by Foreign Gases and Molecular Line Broadening

In astrophysics, the interest in molecular line broadening is actually increasing, owing to the increasing importance of spectroscopic diagnostics in planetary atmospheres and aeronomy. However, from the quantum chemistry point of view, the subject is very difficult and very few scattered results can be theoretically attained. Furthermore the physicists' actual preoccupations are not generally directed towards astrophysical applications except in certain cases. As a matter of fact the elucidation of detailed molecular dynamics is becoming increasingly fruitful, owing to the rapid advances in molecular beam technology which make possible experiments free from macroscopic constraints such as temperature, pressure and impurity concentrations. There is in fact a greater need for an augmenting theory based on the description of detailed dynamics than for results based on traditional pressure broadening theories and on the statistical effects of collisions. In this way a semi-classical approach to spontaneous emission of molecular collision systems has been developed(63): it involves the derivation of a dynamical theory of fluorescence line shapes which is valid for all frequency regimes and not just in the line wings.

In view of stellar atmospheres diagnostics, the broadening and shift of the sodium D lines perturbed by atomic hydrogen have been measured in a combustion driven shock tube(64); the broadening by Ar and H₂ has also been obtained and agrees with previous measurements made in different experimental conditions; for atomic hydrogen, however, these new values differ significantly from the available theoretical results, casting doubt on the validity of the Na-H interatomic potential used in the calculations. The important effort concerning noble gas broadening is continuing: molecular-structure calculations for alkali-metal atom

+ He systems have been performed(65), leading to pseudo-potentials relevant for ground states and numerous excited states: they are in overall good agreement with recent available experimental data, indicating a large improvement on all previous calculations for these systems. Quantum close coupling impact broadening and shift of the D lines of sodium perturbed by He have been performed: the hyperfine components of the same fine structure lines have the same width and shift(66) as expected; the temperature dependence ($800 < T < 4500$ K) has also been studied, and is in satisfactory agreement with available experiments(67). The broadening of resonance lines of Cs by noble gases has been measured at low(68) and high temperatures(69); also concerning Rb ns and nd(70), and Sr 5s ns 1S_0 , 5d and 1D_2 , 3D_2 , by He and Xe(71). Detailed analysis of profiles of the calcium 4227 Å line perturbed by Krypton and obtained by laser induced fluorescence show departures from the usual reduced Voigt form(72). Though far from direct astrophysical application, this paper is quoted there because the obtained profiles show an asymmetry of the Anderson-Talman unified theory type, due to the radiation emitted during the collision: these results emphasize the need for a sophisticated description of the profile when accurate measurements are made in the wings or in the adjacent continuum(73),(74).

Concerning line width parameters in molecular broadening, various results have been obtained: the rotational spectrum of NO₂ at 300 K and $10^{-3} < p < 0.2$ torr has been carried out(75); similarly for CH₃ CN(76). Pressure broadening in the infrared lines of CO($v = 1 \rightarrow 0$) perturbed by H_e and H₂ at liquid nitrogen and room temperature have been measured(77): these data which are of direct astrophysical interest have been compared to *ab initio* quantum calculations: the accuracy of the CO-H_e data have allowed to choose between the two available potential energy surfaces, but the rather poor sensitivity of the pressure broadening to the anisotropic interaction has to be pointed out.

Inspired by the highly successful observations made aboard Voyager I space craft, and ground based high resolution astronomical measurements, a wide ranging series of high resolution (0.04 cm^{-1}) measurements has been performed in the laboratory at NASA Ames Research Center, using an infrared Fourier transform spectrometer. In view of applications to lines formed in Jupiter, Saturn, Titan and Earth atmospheres in mind, N₂ has been used as the broadening gas. Comparisons of observed and computed spectral transmittances have yielded line strengths, N₂ broadened half-widths, and their variation with temperature ($100 \text{ K} < T < 297 \text{ K}$); the measured widths are considerably larger than those used in the AF GL compilation; the ν_4 fundamental band of $^{12}\text{CH}_4$ (78), $^{13}\text{CH}_4$ (79), $^{12}\text{C}_2\text{H}_2$, $^{12}\text{C}^{13}\text{CH}_2$ in the $13.7 \mu\text{m}$ region(80), C_2H_2 in the $7.53 \mu\text{m}$ region(81) and CH_3D (ν_2 fundamental)(82) have been carried out. Other molecules are in progress ($^{12}\text{C}_2\text{H}_4$, C_2H_6 , $^{12}\text{C}_3\text{H}_8$, $^{14}\text{N H}_3$ and $^{15}\text{N H}_3$).

5. Collisional Redistribution of Radiation, Transfer of Radiation and Related Topics

Recent developments in high resolution and high sensitivity spectroscopy and atomic excitation by tunable laser sources have increased the interest in collisional redistribution of radiation and related molecular dynamic studies. They can be divided into two main parts: first, the redistribution of weak radiation field is of direct astrophysical interest; the atom-field interaction can be treated by perturbation theory and induced emission can be neglected. Secondly, the redistribution of strong radiation field, which does not seem to be of direct astrophysical interest, occurs when induced emission is important and when the atom field interaction cannot be treated by perturbation theory: the formalism of the dressed atom has then to be used. In the present report we will focus our attention on the redistribution of weak radiation.

Earlier work based on the unified theory of the redistribution of radiation by collisions for isolated lines has been extended to overlapping lines: and explicit expression for the frequency redistribution has been given for $Ly\alpha$, valid even in the non impact regime(83). Following this work, a consistent formulation for the $H\alpha$, $Ly\alpha$, $Ly\beta$ system is ready to be published(84). It must be pointed out that redistribution in the hydrogen line wings requires a very complicated non-Markovian formulation. Experiments(85) have demonstrated the importance of lower state radiative decay as a mechanism for redistribution in the absence of collisions, leading to the conclusion, contrary to $Ly\alpha$, that complete redistribution may be a good approximation for $H\alpha$.

The fundamental of the formulation of the related topics of radiative transfer and statistical equilibrium equations have been examined. The equations for redistribution have been derived in a quantum mechanical impact framework(86) and the equation of transfer has been derived for broad band fields from Maxwell's equations(87). The effects of stimulated emission in the astrophysical context have been clarified(88) and a work is also in progress on clarification of velocity changing effects.

An attempt to formulate, in a general way, the problem of the transfer of line radiation by multilevel atoms allowing for the effects of partial redistribution has been presented(89); the importance of the knowledge of the distributions of photons and particles is emphasized(90), velocity-averaged line profile coefficients have been considered(91) and explicit expressions have been obtained for a three-level atom in terms of the local radiation intensity field. The concept of the redistribution function has been generalized in the impact framework to other resonance two photon processes including resonance Raman scattering, resonance two photon absorption or emission, and inverse Raman scattering(92).

Farther from astrophysical applications one may quote a number of theoretical works of fundamental interest. A model microfield theory redistribution of intense radiation has been developed(93). Basic studies of the fluorescence spectrum and the probe absorption spectrum of an atom in a radiation field and a sea of binary perturbers have been performed(94),(95),(96).

A non adiabatic theory of atomic neutral line broadening is being developed: the theory of atomic scattering in the presence of a radiation field is used to incorporate simultaneously in the close coupled equations the effects of inelastic scattering and dipole coupling due to the field in an original manner(1),(97),(98). These studies (see also(99),(100)) are relevant both for radiation redistribution studies, radiatively-aided collisions and "half-collisions" analysis of atomic line shapes studies(1),(2). A review paper which concerns this field of research has been written(101) (cf. also the invited talks of (1) and (2) relative to this subject) and evinces the increasing importance of this field of research which appears to be rich in potentialities for future astrophysical applications.

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B. COLLISIONAL CROSS SECTIONS

Because of the magnitude and diversity of material on electron and heavy-particle collisions, I gave references only to published papers of obvious immediate relevance to astronomical research.

1. Electron Collisions

1.1 ELECTRON IMPACT IONIZATION

A valuable compilation of semi-empirical cross sections and rate coefficients for electron impact ionization of a wide range of ions, expressed in convenient analytical form has been prepared(1). An empirical formula for K-shell ionization cross sections was derived(2). Theoretical estimates '233 for the ionization of complex ions were given (3,4). Experimental values were obtained for $Al^+(5)$, He(6), $Fe^+(7)$, Mg^+ , Ca^+ and $Sr^+(8)$, $Be^+(9)$, Ne^{3+} , Ar^{3+} , Kr^{3+} , $Xe^{3+}(10a)$, Mg^+ , Al^{2+} and $Si^{3+}(10b)$, and B^+ , C^{2+} and $O^{4+}(11)$. Ionization rate coefficients were measured for NeVI, NeVII, OVI and Ti IX(12) and for nitrogen ions(13). Distorted wave calculations for the ionization of FeX and the iron ions from FeXV through FeXXVI were reported(14).

2. Electron Impact Excitation

An extensive bibliography of data on electron impact excitation (and ionization) was published(15). Many calculations of excitation cross-sections of varying degrees of sophistication were carried out for positive ions since the last IAU report: Inner shell excitation of helium-like ions(16), lithium-like ions(17a,b) and beryllium-like ions(18) were studied. More detailed calculations were performed for SiIX(19,20), OIV(21), NeV(20,22), CaXV(23), CaXVII(24), SIII(25), SiX(26), SXII(27), OVII(28,29), CV and MgXI(30), SV(31), FeXXV(32), Li-like ions (33), SIII(34), MgVII(35), OII and OIII(36), OIII(37), SII(38), FeX and FeXV-XXVI(14), NeIII(39), NIII(40), FeXX(41), CaXVII(42) and CII(43). Cross sections for excitation to high n states of hydrogenic ions have been obtained using the Born approximation(44). Excitation of hydrogen, helium, lithium and beryllium-like ions has been studied(45) and of sodium-like ions in(46).

Electron impact excitation rates for neutral helium are given in(47-50) and for neutral hydrogen in(51,52). Fits to many excitation rate coefficients are given in(53-55). Studies of excitation to auto-ionizing levels and satellite line emission are described in(56-67). Experimental work on electron impact excitation may be found in(64-68).

A valuable compilation of electron impact excitation rate coefficients of astrophysically interesting systems has been assembled by Mendoza(69) and a useful survey of low energy collisions with complex atoms and ions has been presented by Burke and Eissner(70).