

COMMISSION 14: ATOMIC AND MOLECULAR DATA; formerly: FUNDAMENTAL SPECTROSCOPIC DATA  
(DONNÉES ATOMIQUES ET MOLECULAIRES)

Report of Meeting, 14 August 1976

PRESIDENT: E. TREFFTZ

The first topic of the business session was a discussion on the structure of the Commission. In her introduction the president described the difficulty in serving the astrophysics community with the physical data needed. There are two somewhat contradictory points. On the one hand the Working Groups established by now are not able to pick up new needs of data which come up with new techniques of astronomical observation. On the other hand the material to be covered by the existing Working Groups gets out of hands. The situation is different for the different Working Groups. Working Group 1, Wavelength standards, will be discussed later, it does not pose problems with the material to be covered. The material covered by Working Groups 2 and 4 (Atomic Transition Probabilities and Structure of Atomic Spectra resp.) is the same as that collected by the NBS groups under the same authors, W. Wiese and W.C. Martin. Reference to those well known collections enables the authors to write a useful report within the restricted length allotted to them. For Working Group 5, Molecular Spectra, the material to be covered is blowing up critically because not only the spectral region has been widened to the UV, IR and microwaves, but also transition probabilities are wanted besides the quantities describing the spectra. The worst situation is found in Working Group 3, Collision Cross-sections and Line Broadening. The report can by no means cover all work done during the last three years. It may quote data centres and review articles and then give some examples of present activities. But even then the restriction in length is so pressing that the question arose whether a report like this still makes sense.

The following decisions were taken: Basically the structure of the Commission is useful. The Organizing Committee is asked to enquire what can be done about physical data needed in astrophysics but not supplied by the Working Groups of Commission 14. All members of the Commission who know about such needs should consider how they can be of help (organizing work shops, referring to data centres). About this or if they themselves have collected data they should inform the President of Commission 14, J.G. Phillips, who will mention these activities in the next report. To avoid dropping valuable information because of restriction in length of the report it was suggested by J.G. Phillips to collect the material annually and have it published in some cheap form. The next report can then quote these and restrict itself to a survey and a few highlights.

A suggestion of W.C. Martin to structure the report in table form may also help to make it more useful to astrophysicists. All chairmen of Working Groups agreed that the amount of work put into the report is so high that we should do everything to make it known not only to astrophysicists but also to physicists working in related fields.

Future of Working Group 1, Wavelength Standards. It was found that the primary wavelength standard is mainly dealt with by nonastronomers. This brought up the question whether we should continue the Working Group. To astronomers good secondary standards are of vital interest especially when new spectral regions become available to astronomical observation. K.M. Baird was asked to continue the Working Group, and perhaps suggest the one or the other colleague working in this field to apply for membership to the IAU, Commission 14.

K.M. Baird gave the following additions to his report of Working Group 1, Wavelength Standards (Transactions of the IAU XVII A): (1) The International Advisory Committee for the Definition of the Metre met in June 1979 to consider progress toward a formal redefinition of the metre in terms of the velocity of light. New data were presented and a number of resolutions were passed including a proposed wording of the new definition, and wavelengths of  $I_2$  lines used to stabilize an Argon laser at 515 nm and a He-Ne line at 612 nm. It is expected that a new definition will be approved by the General Conference of Weights and Measures in 1983 (to be reported in Procès Verbaux du B.I.P.M.). (2) An independent (the third) measurement of the velocity of light has just been completed at N.R.C. (Ottawa) yielding a value in agreement with that proposed in 1973 to within a few parts in  $10^{10}$ . As its accuracy was largely limited by the uncertainty in the present  $Kr^{86}$  standard, the result ought to lay to rest any lingering fears that there might be a discontinuity in the length of the metre by adoption of a definition stating  $C = 299792458$  m/s exactly (submitted to Optics Communications).

W.C. Martin gave the following addition to his report of Working Group 4, Structure of Atomic Spectra: The upcoming NBS "Bibliography on Atomic Energy Levels and Spectra" (1) will cover the literature from July 1975 through June 1979. Edlén's paper giving predictions of energy levels and wavelengths for Li I-like ions ( $Z=3-28$ ) has appeared (2), and a similar treatment for the Be I-like ions is in press (3). Recent compilations of atomic energy levels at NBS include Mg I-XII (4), Al I-XIII (5), K I-XIX (6), Ca I-XX (7), and Ti I-XXII (8). The tables for O V in C.E. Moore's "Selected Tables of Atomic Spectra" have been submitted for publication (9). Bashkin and Stoner's "Atomic Energy-Level and Grotrian Diagrams, Vol. II, Sulfur I-Titanium XXII" has appeared (10), and Kelly has compiled the lines of the elements H through Kr over the range 2000-3200 Å (11). Ch. Mogre-Sitterly presented predictions of wavelengths of intercombination lines  $2s^2 2p \ 2p^0 - 2s 2p^2 \ 4p$  of boronlike ions Mg VIII to Ni XXIV which have been determined by B. Edlén.

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Report of Meeting, 15 August 1979

INFORMAL GATHERING AFTER THE JOINT COMMISSION MEETING ON THE COMING SOLAR MAXIMUM  
(COMM. 10, 12, 14, 44)

Since in the four sessions of the Joint Commission Meeting questions of ultra-

violet spectroscopy could scarcely be handled an informal gathering was organized afterwards with R.W.P. McWhirter being chairman.

A.H. Gabriel spoke about "The Observation and Interpretation of the X-Ray Spectrum". The spectrum between 1 and 20 Å is determined largely by the resonance transitions of heliumlike and hydrogenlike ions and their satellites. The satellites are produced near the resonance transition when additional electrons occupy higher orbits, e.g.



Ions of O, Ne, Mg, Si, S, Ca, Fe have been observed. The most prominent satellites are those of the lithiumlike species:  $1s^2nl \rightarrow 1s2pnl$ ,  $n = 2, 3, 4, \text{etc.}$  The levels are populated by dielectronic recombination (inverse autoionization combined with stabilizing radiative transition) and inner shell excitation by electron impact. From the intensity of lines the electron temperature  $T_e$ , the ionization balance  $T_z$  and perhaps even deviation from a Maxwellian distribution of electron velocities may be determined. For that purpose wave lengths  $\lambda$ , radiative transition probabilities  $A_r$ , autoionization probabilities  $A_a$ , and electron impact excitation rates  $C_{is}$  must be known. Groups in Nice (F. Bely-Dubau, P. Faucher, L. Steenman-Clark), Meudon (J. Dubau, M. Loulergue), Mons (S. Volonte), and Culham (A. Gabriel, J.G. Phillips) cooperate on this program. They use the program "Superstructure" of W. Eissner et al. to calculate  $\lambda$  and  $A_r$  taking account of relativistic effects (Breit-Pauli approximation). For  $A_a$  and  $C_{is}$  a distorted wave approximation is used for the electron impacting on a "Superstructure" target. Similar calculations are also done in Moscow by L.A. Vainstein, U.I. Safronova, A. Urnov et al. who use a perturbation expansion in  $1/Z$  ( $Z$  nuclear charge in the target description and charge of the ion in the description of the impacting electron) together with Coulomb radial wave functions. An example shows the satellites of Fe XXV. If the additional electron  $nl$  is highly excited the satellite cannot be resolved from the main line. This must be taken into account in the diagnostics. Work is in progress on Fe XXV, Fe XXVI, Mg XI, Mg XII, O VII, Si XIV, Ca XIX. A special problem is posed by transient ionizing plasmas. Here all the processes mentioned above must be considered, and in addition inner-shell ionization. In the discussion some details of the plasma diagnostics calculations were explained.

G.A. Doschek discussed the solar VUV spectrum  $1000 \text{ \AA} < \lambda < 2000 \text{ \AA}$ . He reviewed density-sensitive spectral line intensity ratios in the 1000-2000 Å region, primarily for lines formed between  $\sim 2 \times 10^4$  K and  $2 \times 10^5$  K. The results are applicable to the solar spectrum and perhaps to other stellar spectra as well. Density-sensitive line ratios involve the ratio of the intensity of an intersystem or forbidden line to the intensity of an allowed line formed in the same plasma region as the intersystem or forbidden line. The ions Si III, S IV, C III, N III, N IV, O III, O IV and O V have metastable levels that give rise to intersystem transitions in the 1000-2000 Å region. For quiet sun densities ( $\sim 10^{10} \text{ cm}^{-3}$ ) only the C III 1909 Å line is useful for density determinations. For solar active regions and flares,  $N_e \geq 10^{11} \text{ cm}^{-3}$ , many of the lines of the other ions are useful. Two techniques were discussed and compared: (1) using the intensity ratio of an intersystem line of one ion to the intensity of an allowed line of a different ion, and (2) using the intensity ratios of two lines arising from the same ion. The effect of density on intersystem and allowed line profiles was outlined. The theory was illustrated with spectra recorded by the NRL slit spectrograph flown on Skylab. A density-sensitive line ratio of S X was also discussed. S X is formed at about  $1.3 \times 10^6$  K, so this diagnostic is useful for coronal plasmas. The S X lines appear near 1200 Å and are strong lines in Skylab spectra obtained outside the solar limb. Finally, the He II 1640 Å line profile observed in quiescent prominence spectra was shown. This line is formed at about 25,000 K. It was suggested that the excitation mechanisms of the fine structure components be investigated in detail for possible application to solar or stellar atmosphere problems.

H. Nussbaumer described the methods used to meet the needs for atomic data. He described the basic quantum-mechanical approaches and the criteria for accuracy. The latter are supplied by measured energy levels. For many astrophysically important ions, especially those of carbon, nitrogen and oxygen and their isoelectronic series a simple self-consistent-field approach is insufficient. A configuration expansion improves the results considerably. Judging the accuracy of transition probabilities is difficult. Most error estimates are hardly more than guesswork. Exact error bounds exist, cf. F. Weinhold, 1971, *J. Chem. Phys.* **54**, 1874, but unless the wave functions are very good the bounds are too wide to be of practical use. In the isoelectronic sequence of Be I different high quality calculations agree now within 3%. The discrepancy to measurement of C III to Ne VIII is less than 20%. For the intercombination transition  $2s^2\ ^1S_0 - 2s2p\ ^3P^o_1$  of C III a detailed error analysis was given which leads to a transition probability of  $96 \pm 11\ \text{sec}^{-1}$  with the largest uncertainty,  $6.4\ \text{sec}^{-1}$ , coming from spin-orbit splitting. The effect of uncertainties in the transition probabilities on the plasma diagnostics was shown for the O IV intercombination system: If new A values differ by 50% in absolute value but only by 10% relative to each other the electron density  $N_e$  inferred from intensity ratios is changed by a factor of 2.

Collision cross sections of those ions show a lot of structure. Below each excitation threshold a Rydberg series of resonances occurs. In Coulomb Born approximation these are neglected. Also the Distorted-Wave approximation which replaces the Coulomb potential by a refined ion potential neglects them. Close-Coupling calculations take them into account. But it should be kept in mind that the quality of the results depends sensitively on the quality of the target description and on a sufficiently high number of partial waves (characterized by the angular momentum of the impacting electron) taken into account. The electron impact excitation of Fe VI was shown as an example.

In the discussion C. Jordan mentioned a problem with the high excitations in Si VIII and Fe XII. Answering a question of E. Trefftz she does not think it to be an effect of dielectronic recombination. H. Nussbaumer explained his error estimate of the C III intercombination transition probability in some more detail.

#### Report of Meeting, 17 August 1979

#### MOLECULAR DATA

The following additions to the reports in Transactions of the IAU, Vol. XVII A were given: Working Group 5, Molecular Spectra. R.W. Nicholls announced that the book of Huber and Herzberg (1) has appeared. He mentioned the compilation of CNRS (2) and two review papers on the systematics of molecular intensities which R.A. Hefferlin has found in the Soviet journals *Uspekhi* and *Optics and Spectroscopy*. G. Herzberg (3) reports a new spectrum in discharges in  $H_2$  and  $D_2$  which can be definitely ascribed to transitions between Rydberg states of  $H_3$  and  $D_3$ . It results from one of the radiative channels of the dissociative recombination of  $H_3^+$  and  $D_3^+$ . J.W. Brault reports on the interferometer mounted at the Kitt Peak solar telescope. It can be used in an astronomical or laboratory mode. Recent laboratory work has been on  $CH_4$  and  $HCHO$ . The free spectral range of this instrument is 2000A-10 $\mu$ . It has a resolving power of  $2.5 \times 10^6$ . Its wavelength precision is 1 in  $10^9$  and the signal to noise ratio is in the  $10^4$ - $6 \times 10^4$  range. R.W. Nicholls has done some recent theoretical work to model photodissociation phenomena (4).

P.K. Carroll described work on the complex spectrum of FeH in the blue, green and infra-red regions out to beyond 9000 Å. Work was also reported on the 3678 Å band of CrH, a molecule which has been found in cool stars by Lindgren and others through the Keenan band at 8611 Å. Work is also in progress on the CO spectrum from 800 Å to 1200 Å using plates taken at Ottawa and about 100 bands have so far been analysed.

P.L. Smith reported work on the oscillator strengths of lines likely to be seen in interstellar clouds. These include lines in the  $\tilde{C}-\tilde{X}$  and  $\tilde{F}-\tilde{X}$  bands of H<sub>2</sub>O near 1240 Å and 1115 Å, respectively, and also the line R(0) of the C-X band of HCl at 1290 Å. These lines have not yet been found in interstellar sources.

B. Petropoulos reported work on Franck-Condon factors by the RKR method for the A-X system of CO, and results of the application of this work to the study of the spectrum of Mars.

S. Sahal presented additions to the printed Report on line broadening. For Stark broadening she indicated a general agreement between theory and experiment of 20 to 30 per cent. New work was available by F. Praderie and H. Hubeny for the Lyman alpha line in Vega. She discussed the formation of eximers and collisional broadening in the far wings of atomic lines. J. Cooper has studied the problem of the redistribution of radiation, but the case of the hydrogen lines still needs to be done. There is still a need for improvements in collisional broadening for molecular lines for planetary atmospheres applications.

E. Trefftz drew attention to the Chemical Kinetics Data Center at NBS Washington. She mentioned recent work on charge exchange at the Lebedev Institute, Moscow, and a talk given at the Max Planck Institute by A. Luntz, IBM San Jose Research Lab, on the excitation of oxygen atoms by impact with hydrogen molecules and hydrocarbons.

J.G. Phillips drew attention to the large number of papers on electron impact on molecules, with some 72 papers on 28 molecules during the last year or so. Most papers have been on H<sub>2</sub>, and CO<sub>2</sub> and N<sub>2</sub> have also been extensively studied, mostly by ab initio calculations. There have also been many papers on photoionization. A supersonic nozzle has been used to give excitation temperatures of 10 to 30° K, which has made some experiments easier.

W. Huebner pointed out that at temperatures of a few thousand degrees Kelvin, and at low density the Rosseland mean opacity of hydrogen is dominated by the total extinction on the far red side of Ly α. It is important to have a theoretical model and measurements of the absorption and scattering properties of atomic hydrogen for photons with energy between about 1 and 9 eV.

J.H. Black gave a review of the highlights of I.A.U. Symposium No. 87 on Interstellar Molecules, which had been held prior to the main I.A.U. General Assembly. Molecules are important as diagnostic tools, including searches for isotopes, and searches for unusual species. 52 interstellar molecules have been observed, 13 inorganic and 39 organic, including one with 11 atoms and four with 9 atoms; no ring molecules have been identified. Species first seen in space are HCO<sup>+</sup>, C<sub>2</sub>H, N<sub>2</sub>H<sup>+</sup>, C<sub>4</sub>H and C<sub>3</sub>N. About 185 radio frequency interstellar lines remain unidentified. Many molecules appear to be formed in large networks of reactions; many reaction rates are known at room temperatures but they have not been measured at 20° K. Associative reactions such as C<sup>+</sup> + H<sub>2</sub> → CH<sub>2</sub><sup>+</sup> + hv and CH<sub>3</sub><sup>+</sup> + H<sub>2</sub> → CH<sub>5</sub><sup>+</sup> + hv are important as the starting points of chains of reactions, for example the second of these reactions may lead to CH<sub>4</sub> and H<sub>2</sub>CO, among others. Statistical theory and experiment applied to the corresponding three body reactions suggests which processes are likely to be rapid. High temperature chemistry may also be important;

observations of the  $H_2$  quadrupole radiation in the Orion cloud lead to a kinetic temperature of  $2000^\circ K$ . At high temperatures many more reactions are possible. Among specific processes, the photodissociation rate of  $CH^+$  is larger than formerly thought. Oka is working on collisional excitation of molecules by  $H_2$ , and it matters whether  $H_2$  is in para ( $J=0$ ) or ortho ( $J=1$ ) state. The astronomical rate of  $H^+ + O \rightarrow O^+ + H$  has been confirmed theoretically. There are many challenges to experimenters. Predictions suggest that  $C^+ + H_2 \rightarrow CH_2^+ + hv$  is fast, and that  $Cl^+ + H_2 \rightarrow HCl^+ + H$  may be slow at low temperatures. Isotopes continue to be of interest, refined abundances of isotopes are important as constraints on nucleosynthesis. HDCO has now been detected: it is probably formed by gas phase reactions. On the observational side, radio identifications of lines may be nearing the confusion limit. Infrared techniques are developing rapidly. Prospects are dim for studies of  $H_2$  below  $1100 \text{ \AA}$ , even the Space Telescope will have poor response at that wavelength. The most pressing needs at present are for further spectroscopy to aid in identifications, measurement of reaction rates especially at low temperatures, rates for radiative association processes, and further study of collisional excitation mechanisms.

G. Herzberg mentioned that in addition to the new Rydberg spectrum of  $H_3$  and  $D_3$  he had also found a related spectrum in  $NH_4$  and is trying to find one for  $CH_5$ . It may shed light on the dissociative recombination of  $CH_5^+$ . From radio observations it looks as though the abundance of  $CH_4$  must be enormous. The question of how much CO and C is tied up in grains is hard to answer.

W. Huebner described his calculation of model comae of comets. The gas density just above the surface of the vaporizing icy nucleus of a moderately active comet at 1 AU heliocentric distance is several times  $10^{13}$  molecules per  $cm^3$ . The gas streams outward at first with a speed of  $\sim 0.1 \text{ km/s}$  but rapidly reaches its terminal, supersonic speed of  $\sim 1 \text{ km/s}$ . Its initial temperature is typically  $150$  to  $200^\circ K$ . Solar uv radiation penetrates to  $\sim 100 \text{ km}$  of the nucleus (at 1 AU) dissociating and ionizing the gas. It has been found that photodissociative ionization plays an important role in the inner coma, producing radicals and ions that fuel a complex chemical reactions network in which new species are formed that are not simple decay products of the initial vaporizing gas. Over 600 reactions of 100 species are included in the model, and time dependent solutions are obtained. The relative importance of various reactions changes with the distance from the cometary nucleus, so that it is difficult to simplify the network of reactions. Many species do not reach chemical steady states. A large number of photo rates in sunlight at 1 AU heliocentric distance have been computed for atomic hydrogen, carbon, nitrogen, and oxygen and for some molecules formed from these elements. Most urgently needed are branching ratios for photolysis and for chemical reactions. A problem of the present model is that we still cannot produce enough  $C_3$ .

Answering a question W. Huebner pointed out that the most needed observations are those of column densities of the various species at well defined positions of the line of sight with respect to the nucleus. A special problem is posed by the  $H_2O^+/CO^+$  ratio.

A.J. Sauval spoke on molecular data needs for cool stars. A survey of physical parameters of the different types of stars shows that they may serve as a laboratory of molecular spectroscopy. Temperatures and column densities are higher than in ordinary laboratory conditions. For some stars the spectrum is extremely stable, equilibrium conditions are well satisfied. Disadvantages of the stellar lab are the temperature stratification, the complicated and unknown chemical composition which yields blends, perturbations (motions, magnetic fields), and absorption in the earth's atmosphere. Of the molecules identified so far in the UV - Visible - IR about 80% are diatomic compounds of H and O. Polyatomic molecules of H, C, N, O (Si, S) are mainly observed in the microwave region and the Infrared ( $\lambda \gtrsim 3\mu$ ). Circumstellar envelopes which give rise to radio emission lines are not in thermal

equilibrium (OH, SiO, H<sub>2</sub>O). A list of observed transitions shows how many data are still lacking - oscillator strengths, Franck-Condon factors, - even for known spectra. The abundance of a molecule depends on the abundance of its components and on its dissociation energy. This explains the high interest in hydrides and monoxides. But also monocarbides, -nitrides, fluorides and sulphides deserve laboratory study. Especially poor is the knowledge of positive molecular ions. Of metal compounds most prominent are titanium and zirconium compounds. Also here spectra and dissociation energies are lacking for some compounds. The situation for other metals is even worse. In S stars the number of free carbon and oxygen atoms is a sensitive test for the abundance ratio  $n_C/n_O$  since the less abundant atom is almost completely bound in molecules. Regularities between isoelectronic sequences of molecules may help clarifying the spectra. After describing new results for TiO and ZrO a long list of wanted work on spectra, classification of bands and rotational analysis was presented (list still available to the author).

W. Huebner asked whether the assumption of chemical equilibrium is justified in a stellar atmosphere. That is an approximation, but owing to the high temperature and the large density it surely is much better justified in stars than in comets or in the interstellar medium.

K.H. Hinkle, Kitt Peak National Observatory, discussed high resolution infrared stellar spectroscopy and its data needs. The development of Fourier Transform Spectrometers (FTS) and increasingly sensitive infrared detectors have made a large number of astronomical sources available for high resolution ( $\Delta\lambda/\lambda \gtrsim 2 \times 10^{-5}$ ) spectroscopy in the 1 to 5  $\mu$  infrared. Currently, the FTS at the coudé focus of the 4m Mayall telescope at Kitt Peak National Observatory has obtained high resolution, high signal-to-noise spectra to K magnitude +4 and M magnitude -1. The K magnitude limit is about one magnitude fainter than the limit for the 2 $\mu$  Infrared Catalog, implying that nearly 10,000 objects are bright enough to be observed at high resolution. The FTS has also achieved very high resolution (up to 0.006  $\text{cm}^{-1}$ ) for the brightest sources. In order to interpret high resolution, infrared spectra of astronomical sources, high quality laboratory spectra are needed. Astronomical infrared spectra in the 1 to 5 $\mu$  region are dominated by vibration-rotation transitions of light molecules including CO, OH, H<sub>2</sub>O, SiO, C<sub>2</sub>, HCN, C<sub>2</sub>H<sub>2</sub>, CS, CH, NH, H<sub>2</sub>, HCl, and HF. The 0-2 and 0-1 sequences from the  $A^2\Pi-X^2\Sigma$  transition (red system) of CN and atomic lines, particularly from metals of atomic weight near Fe, are commonly found in infrared spectra. Exceedingly large column densities (up to  $\sim 10^{26} \text{ cm}^{-2}$  for H<sub>2</sub>) can be observed in cool stellar atmospheres. Since typical excitation temperatures are near 3000K, lines of high excitation can be found in stellar spectra. For CO laboratory frequency measurements extend to  $J'' \sim 90$  while even in the relatively CO weak KO giants the 2-0  $J'' = 90$  line has a central depth of about 10% and 2-0 lines of  $J'' \gtrsim 110$  can be identified. A few molecules are in desperate need of improved measurements. NH is a potentially important nitrogen abundance indicator. Its fundamental vibration-rotation band which is present in 4 $\mu$ m region spectra of the M supergiant  $\alpha$  Ori, has no frequencies or oscillator strengths measured in the laboratory. The elements Sc, Ti, V and Ni contribute a number of strong lines in the 2-5 $\mu$ m infrared spectra of stars. Both accurate laboratory frequency measurements of these lines and identifications of any weaker lines of these elements present in infrared spectra are urgently needed.

E.E. Whiting introduced a discussion on the rotational line intensity factors for diatomic molecules (Hönl-London factors) and the different normalization schemes in use for them. Uncritical use of published values of Hönl-London factors in ignorance of the normalization used for them can lead to grave errors. Together with J.B. Tatum and R.W. Nicholls he advocated a unique convention on a normalization which is self-consistent. It was agreed to draft a statement incorporating the recommended convention and to circulate it for consideration to the Inter-Union Commission on Spectroscopy (IUCS which has 3 representatives from IAU, 4 representatives from IUPAP and 4 representatives from IUPAC).

F. Remy reported lifetime measurement of electronic states in molecules. In the evaluation of the decay curves care must be taken to account properly for repopulation by long living states. A mere a priori subtraction of a so-called experimental background (determined by a blank experience) may lead to large errors. An attempt to use the dependence of the lifetime on the vibrational quantum number to determine the variation of the electronic transition moment with the internuclear distance is not successful owing to errors in the measured lifetimes. Large discrepancies in the published values of the  $N_2C^3\Pi_u$  lifetime are due to radiation trapping between this state and the long lived upper state  $B^3\Pi_g$  of the first positive system.

R. Clegg discussed the unidentified Keenan bands in the 8000 to 11000 Å regime of S stars. Accurate band head wavelengths have been observed. High resolution (0.4 Å) spectra do not resolve the rotational structure indicating that the molecules are not hydrides. The 8610 Å band is not due to CrH. Spectroscopic data and chemical equilibrium calculations restrict the list of candidate molecules. Laboratory spectroscopy is wanted for: ZrS, CeS, ZrCl, YCl, LaCl, CeCl, ZrOH, LaOH, CeOH, YOH, for LaS ( $\lambda > 0.9\mu m$ ) and for ZrO, CrO, NbO ( $\lambda > 1\mu$ ). Two new transitions of CeO have been seen in R Gem. In the same star LaO explains part of some bands.

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Report of meeting, 20 August 1979

#### ATOMIC DATA

The last session of the Commission started with some business. The Organizing Committee, the Chairmen of the Working Groups, the new members of the Commission were announced. There being no objection, all names were accepted. The president reported that the Organizing Committee was proposing a change of name of the Commission. The new name will be "Atomic and Molecular Data". Considering an objection of Ch. Moore-Sitterly that the new name opens the door to unreliable data the Organizing Committee felt that the chairmen of the Working Groups could deal with this danger, that on the other hand non-spectroscopic data are needed in astrophysics and handled by Commission 14. These data are by nature less reliable. The new name describes the activities of Commission 14 more properly than the old one. The suggestion of J.G. Phillips (our next president) to collect material for the report annually was accepted for a try.

W. Wiese's addition to the report on Atomic Transition Probabilities were presented by W.C. Martin: A compilation of transition probabilities for selected lines of H through Ni has appeared in the CRC Handbook of Chemistry and Physics (1). Transition probabilities for doubly-excited states of He I have been compiled (2). Calculations for several Be-like ions have been reported (3,4). Transitions involving doubly-excited states of Be-like ions have been treated (5), and of Fe XXIV (6). Transition probabilities of forbidden lines within the ground configuration of C-like



ions have been calculated (7). Numerous allowed and forbidden transitions of Fe XXI have been treated (8). Lifetimes of excited states have been measured by various investigators, using the Hanle-effect technique in Mg I and Sr I (9), and in In I (10); stepwise laser excitation has been employed in Hg I (11), as well as in Li I (12). Oscillator strengths for lines of the principal series in Rb I have been measured in absorption. (13). Branching ratios for several lines in neutral oxygen have been measured in a hollow cathode discharge (14).

In reply to a question W.C. Martin said that the compilations on wavelengths, energy levels, transition probabilities, ect. were available from him or from Dr. R. Zalubas, A 167 Physics, National Bureau of Standards, Washington D.C. 20234.

Additions to A. Burgess' report on electron impact on and photoionization of atoms and atomic ions were presented by M.J. Seaton. He reported photoelectron spectra of atomic barium by R.A. Rosenberg et al., Lawrence Berkeley Laboratory, to be published.

J.L. Culhane reported on stellar X-ray spectroscopy. The solar X-ray emission spectra has helped in understanding the hot plasma in active regions and in solar flares. The history of the theoretical calculations and of the observations of the coronal X-ray spectra are familiar. Observations of stellar spectra are done e.g. at Naval Research Laboratory (NRL), Aerospace, Lockheed in USA, Mullard Space Science Laboratory (MSSL), Leicester in the U.K. Although the early dispersive spectrometers did not have much success, lower resolution non-dispersive spectrometers have since 1972 been discovering X-ray emission and absorption features in supernova remnants (SNR's), binaries, active stars, interstellar medium, clusters of galaxies, active galaxies. In the observed objects the low resolution spectra have allowed us to identify the following physical situations. SNR's show a shock heated interstellar plasma of a temperature of  $T_e \sim 10^6$  to  $5 \times 10^7$  K and a density  $N_e \sim 0.1$  to  $10 \text{ cm}^{-3}$ , similar to a coronal plasma, and probably not in ionization equilibrium. Some accretion powered X-ray binaries have a photoionized stellar wind. The temperature is  $T_e \sim 10^5$  to  $10^6$  K, but ionization stages up to Fe XXVI exist due to X-ray radiation. The density is  $N_e \sim 10^{11}$  to  $10^{13} \text{ cm}^{-3}$ . One sees emission lines due to fluorescence and recombination and also photoelectric absorption edges. Stellar soft X-ray sources are stars with coronae and winds, and accreting white dwarfs. The temperature is  $T_e \sim 10^5$  to  $10^7$  K, the density  $N_e \sim 10^8$  to  $10^{13} \text{ cm}^{-3}$ . Seen are multi-temperature coronal type emission lines and photo-electric absorption edges. Spectroscopy of extragalactic X-ray sources has indicated that clusters of galaxies have a gravitationally heated intra-cluster medium. This is primordial material enriched by ejecta from galaxies.  $T_e \sim 10^8$  K,  $N_e \sim 10^{-3}$  to  $10^{-4} \text{ cm}^{-3}$ . Cooler material is found around some galaxies. We see multi-temperature coronal type emission lines. Active galaxies are very luminous with an X-ray flux  $L_x \sim 10^{45}$  to  $10^{46} \text{ erg sec}^{-1}$ . The radiation comes from nuclear X-ray sources surrounded by photoionized material. Emission lines due to fluorescence and recombination are seen as are the photo-electric absorption edges. In NGC 4151 and NGC 5128 neutral iron is observed. The following survey of observations refer to the cases mentioned above. Observations of supernova remnants were demonstrated by spectra on Cas A and Tycho taken by Ariel V, Einstein SSS (Holt et al.). Spectra of Pup A observed by rocket (Culhane et al.) and by the MIT satellite (Canizares et al.) show two different temperatures. A suggestion by Itoh explains the low temperature ions by a departure from ionization balance. Spectra of X-ray binaries were shown for Vela X-1 (OSO-8) and Cyg X-3 (OSO-8, Ariel V) and for Capella (HEAO A2 experiment and the Einstein observatory). The latter comprises a G 5 III - G 0 III spectroscopic binary with a period of 104 days. Spectra show Fe XVII and Fe XVIII, Mg XI, Si XIII, S XV. The elements Fe, Mg, Si, S appear to be over-abundant by a factor 1.5 to 6 compared to solar. The X-ray flux is consistent with a magnetic field  $B_{CAP} \sim 10 B_\odot$ . The apparent over-abundance may be explained by a coronal loop structure with different temperatures. With respect to extra-galactic objects the most exciting Uhuru result were extended cluster X-ray sources. Fe XXV, XXVI lines resolved by Ariel V indicate  $T \sim 7 \text{ keV}$

and cosmic abundance. Also  $n = 3$  to  $n = 1$  transitions of these ions are seen and faintly S XV. Einstein SSS observations (Holt et al.) of NGC 1275 confirm the presence of cooler material surrounding NGC 1275. O VIII resonance lines were observed by the MIT-FPC satellite (Canizares et al.) from M 87 in Virgo, indicating a temperature of  $2 \times 10^6$  to  $10^7$  K while the intercluster temperature in Virgo is 30 to  $40 \times 10^6$  K.

Regarding the necessary atomic physics work, it is at present the case that cross-sections and rates appropriate to coronal plasmas are being used to interpret the new data described above. This is acceptable for the present since the spectra are mainly of low resolution and are statistically weak. However the much wider range of plasma conditions (temperature, density, optical depth) that will be encountered in cosmic plasma could show a need for improved data.

R.H. Garstang gave an account of the behaviour of atoms in high magnetic fields, and referred to his review (15). High fields have become of particular interest because of the discovery that certain white dwarf stars show megagauss fields (these stars have been discussed in a review by J.R.P. Angel (16)). Recently it has been suggested that  $C_2$  may be the origin of a very strong absorption feature in the magnetic white dwarf star LP 790-29 (17). Further calculations are clearly needed on the effects of high magnetic fields on molecular spectra, and there is also a need to carry the calculations on simple atomic spectra to higher accuracy and to higher fields.

S. Sahal gave a short account of her work (together with J.L. Leroy, G. Ratier, V. Bommier) on the use of the Hanle effect for determination of magnetic fields on the sun's surface. The strength and direction of magnetic fields influences the degree and direction of polarization of the solar radiation. The case of a prominence on the solar limb was treated in detail. To determine the polarization which would be seen without field a model must describe the excitation mechanisms of the observed spectral line. For symmetry reasons the polarization without field is parallel to the limb. The observed polarization in the line is smaller and rotated by an angle of some  $10^\circ$ . This reduction together with the rotation angle allows the determination of two components of the field. The observation of several lines would allow the complete determination of the magnetic field. Diagrams have been calculated for easy determination. The helium line  $D_3$  was used as an example (18).

C. Jordan mentioned work by S. Johansson, Lund, on the spectrum of Fe II which she is using. She stressed the need for additional oscillator strengths for Fe II in the ultraviolet and for data on polarizability needed for the interpretation of motional Stark effect.

C. Cowley notified the Commission of a new Newsletter on Ap stars, distributed by W. van Rensbergen. There is still a need for oscillator strengths of transition elements such as Ti I, Cr I to which D. Locanthi added Zr I. Damping constants are also needed.

M. Malinowski reported her calculations of intensities of Fe IX, X, XI lines in coronal and laboratory plasmas describing the different processes that had to be taken into account.

P.K. Carroll described work on a plasma produced by a ruby laser. Heavy elements (Mo to U) are up to 16 times ionized. The 40 to 200 Å region was observed. Open d shells give an enormous number of lines which can't be resolved. They form a quasi-continuum.

The president thanked all the Commission members for their interest in the work of the Commission. Special thanks are due to R. Garstang who has served in the Organizing Committee for 5 terms or 15 years and who is now retiring, and to

the chairmen of Working Groups and those who helped preparing the report, to all the speakers for their contributions and all those who participated in the discussion.

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