COMMISSION 36: THE THEORY OF STELLAR ATMOSPHERES (LA THEORIE DES ATMOSPHERES STELLAIRES)

Report of the Meetings on November 20th, 21st and 27th

BUSSINESS SESSIONS

November 20th, 9.00 - 9.20 and November 27th, 11.00 - 11.25

CHAIRMAN: B. Gustafsson SECRETARY: R. Wehrse

I. COMMISSION ACTIVITIES

The President outlined the activities of the Commission in the period following the 18th General Assembly.

II. NEW MEMBERS

The membership of the following 28 new members was approved:
S. Baird, D.N. Brown, K.L. Chan, P. Chen, S. Drake, D. Dravins, J.M. Fontenla, W.R. Hamann, U. Heber, H. Herold, T.H. Kaduri, A.P. Linnell, C. Liu, J. Madej, S. Massaglia, Å, Nordlund, R. Pallavicini, M.G. Rovira, G. Scharmer, W. Schmutz, K.P. Simon, L. Snezhko, H. Spruit, P. Ulmschneider, T. Watanabe, R. White, L.A.Willson, H. Wöhl.

III. NOMINATION OF PRESIDENT AND VICE PRESIDENT

The nomination of K. Kodaira as President and of D.F. Gray as Vice President was approved unanimously.

IV. ORGANIZING COMMITTEE

The following names for the new Organizing Committee were approved:
J. Cassinelli, L. Cram, B. Gustafsson, A.G. Hearn, I. Hubeny, W. Kalkofen, R. Kudritzki, D. Mihalas, M. Seaton, A.B. Underhill.

V. ENDORSEMENT OF RESOLUTION

The Commission endorsed a resolution in favour of the continuation of solar and stellar research activities at Mt Wilson Observatory.

VI. FUTURE ACTIVITIES

The President outlined the planned activities, which were subsequently discussed.

SCIENTIFIC SESSIONS

1) MEETING: November 20th, 9.20, continued on
November 27th, 11.25 - 11.45

Radiative Transfer Chairman: W. Kalkofen

Papers on the following subjects were given:

G.B. Rybicki: The physical principles underlying escape probability methods in radiative transfer.

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R. Wehrse: The generalization of the formal solution of the scalar transfer equation to the set of coupled equations occuring in radiative transfer, subject to integral constraints.

A. Peraiah: The discrete space theory for the solution of the partial differential equation, describing the radiative transfer in an atmosphere with spherical symmetry.

W. Kalkofen: An operator perturbation method employing differential equations for the solution of the radiative transfer equation in conservation form of a two-level atomic model with complete redistribution.

D. Mohan Rao: Time-dependent, multi-dimensional radiative transfer in stellar atmospheres. (Work for a thesis under the supervision of A. Peraiah at Bangalore University).

K.E. Rangarajan: Spectral line formation in stellar atmospheres. (Work for a thesis under the supervision of A. Peraiah at Bangalore University).

Most of the papers presented will appear in a book under the title "Numerical Radiative Transfer", to be published in 1986 by Cambridge University Press. Reviews of numerical methods can be found in "Progress in Stellar Spectral Line Formation Theory", from a conference held in Trieste in 1984, in "Methods of Radiative Transfer", from a session of Commission 36 at the IAU meeting in Patras, Greece, in 1982, and in a review paper by Auer (1986).

The main topics treated at the session in Delhi and in "Numerical Radiative Transfer" are operator perturbation methods and problems encountered in their efficient use, and the transfer of polarized radiation. Additional discussions concern escape probability methods and line blanketing.

References

Methods in Radiative Transfer, 1984, W. Kalkofen ed., Cambridge University Press, Cambridge, UK.

Progress in Stellar Spectral Line Formation Theory, 1985, J.E. Beckman & L. Crivellari eds., D. Reidel Publ. Co., Dordrecht, Holland.

Numerical Radiative Transfer, 1986, W. Kalkofen ed., Cambridge University Press, Cambridge, UK.

Auer, L.H.: 1986, Methods in Comp. Phys., in press.

2) JOINT SESSION (with Commissions 25, 29 and 45): November 20th, 14.00

Synthetic Photometry Chairman: R. Buser

The minutes of this session are published in Highlights of Astronomy, Vol 7.

3) JOINT SESSION (with Commission 14): November 21st, 16.00

Atomic and Molecular Data for Studies of Stellar Atmospheres Chairman: A.H. Gabriel

ATOMIC DATA FOR ANALYSING EARLY-TYPE STELLAR SPECTRA

A.E. Lynas-Gray, Dept. of Physics and Astronomy, University College London.

Among the atomic data needed, for analysing early-type stellar spectra, are oscillator strengths and photoionization cross-sections for the prediction of line strengths together with continuous and line opacities. Electron collision excitation and ionisation rates are also needed if an attempt to solve the radiative transfer equation, simultaneously with the statistical equilibrium equations, is to be made. Some indication of the atomic data that has become available since 1982 is presented below; no attempt has been made to provide a complete bibliography.

A useful review of atomic data, with assessment, available before 1982 has been prepared by Mendoza (1983). Precision oscillator strengths can now be used to obtain large numbers of moderately accurate oscillator strengths, from line intensities (Cowley 1983, Cowley & Corliss 1983) and Kurucz & Peytremann's (1975) tabulation (Blackwell et al. 1983). Variational wavefunctions have been used by Kono & Hattori (1984) to calculate accurate oscillator strengths for neutral helium.

Saraph (1985) has reviewed recent work on photoionization cross-sections. It should be noted that detailed resonance structures have not been incorporated into model atmosphere calculations so far. Bell et al. (1983) have provided recommendations for ground-state electron collision ionisation cross-sections, though the Montagne et al. (1984) recommendation should be adopted for neutral helium. Aggarwal (1983), Aggarwal et al. (1984) and Cochrane & McWhirter (1983) have recommended electron collision excitation cross-sections and rates for HI, He I and Li-like ions, respectively.

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Kurucz, R.L. and Peytremann, E.: 1975, SAO Special Report 362.
Mendoza, C.: 1983, IAU Symposium 103, 143.
Montagne, R.G., Harrison, M.F.A. and Smith, A.C.H.: 1984, J. Phys. B : At. Mol. Phys. 17, 3295.
Saraph, H.E.: 1985, Proceedings of CCP2/CEC Atomic Data Workshop (in press)

COMMENT BY W.L. WIESE:

In addition to the recent data sources on transition probabilities of Fe I cited in the preceding paper, the 1981 data tables by J.R. Fuhr et al. (J. Phys. Chem. Ref. Data 10, 305-565) are worth noting. The significance of these transition probability tables is that all data are critically evaluated and the roughly 2000 selected transitions are estimated to have typically accuracies within the 25 to 50% range and sometimes much better.

COMMENT BY C. COWLEY:

First of all let me say that astronomical spectroscopists owe a great dept of gratitude to Dr. Wiese and his group for their compilations of critically evaluated oscillator strengths for a large number of lines of astrophysical interest. These values provide a world-wide standard to be used in the analysis of cosmic plasmas. I do not see how we could do our research without them.

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I judge from his comment that we still have not clarified the point that we have massive needs that extend beyond these critical evaluations. Our light sources are so powerful, and so contaminated (relative to a good laboratory experiment) that we need data even for lines that have not yet been seen in the laboratory.

This is the reason for our efforts to make use of the Meggers, Corliss, and Scribner TABLES OF SPECTRAL LINE INTENSITIES, as well as the Corliss-Tech work on Fe I (NBS Monograph 108). An immense effort was put into this same basic Fe I data set by Boyarchuk and Savanov (Izv. Crimean. Astrophys. Obs. Vol 70). The new volume of Critical Evaluations by the NBS will contain some 1950 Fe I lines, and will certainly ease the need for reliance on the older systems of measurement. Modern measurements have still not exceeded in number the 3288 Fe I lines of Corliss and Tech, and in the domain of the rare earth lines, there are only a few hundred modern measurements, so our need of Monograph 145 remains strong.

THE EFFECTS OF ATOMIC-LINE ABSORPTION ON STELLAR ATMOSPHERES

R.L. Kurucz, Harvard-Smithsonian Center for Astrophysics

In 1983, working with Lucio Rossi from Frascati and with John Dragon and Rod Whitaker at Los Alamos, I finally completed line lists for all diatomic molecules that produce important opacity in G and K stars. Once the line data were ready, I computed new distribution function opacity tables. The calculations involved 17,000,000 atomic and molecular lines, 3,500,000 wavelength points, 50 temperatures, and 20 pressures, and took a large amount of computer time.

As a test the opacities were used to compute a theoretical solar model, to predict solar fluxes and intensities from empirical models, and (with fudging) to produce improved empirical models that are able to match the Ca II H and K line profiles and both the UV and IR intensities formed near the temperature minimum. The work on empirical models is in collaboration with Avrett and Loeser.

There are several regions between 200 and 350 nm where the predicted solar intensities are several times higher than observed, say 85% blocking instead of the 95% observed. The integrated flux error of these regions is several per cent of the total. In a flux constant model this error is balanced by a flux error in the red. The model predicts the wrong colors. After many experiments with convection and opacities, and after synthesizing the spectrum in detail, I have determined that this discrepancy is caused by missing iron group atomic lines that go to excited configurations that have not been observed in the laboratory. Most laboratory work has been done with emission sources that cannot strongly populate these configurations. Stars, however, show lines in absorption without difficulty.

I have used Bob Cowan's Hartree-Fock programs at Los Alamos to compute Slater single- and configuration interaction integrals for the lowest 50 configurations of the first 10 stages of ionization for elements up through Zn and for the first 5 for heavier elements. These calculations allow me to determine eigenvectors by combining least squares fits for levels that have been observed with computed integrals (scaled) for higher configurations. Each least squares iteration takes a significant amount of time on a Cray and many iterations are required. Thus far I have completed new line lists only for Fe I and II, but they produce the strongest effect on the spectrum. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line. The complexity of these calculations is illustrated by this table,

	Fe I		Fe II	
	even	odd	even	odd
number of configurations	26	20	22	16
number of levels	5401	5464	5723	5198
largest Hamiltonian matrix	1069	1094	1102	1049
number of least squares parameters (many fixed at scaled HF)	963	746	729	541
total number of lines saved	583,814		1,112,322	

I have computed the blocking in the solar ultraviolet spectrum produced by Fe lines, once with the old line data mentioned above, and again with the newly calculated data. The increase in opacity is dramatic. Many moderate strength lines appear to fill in the gaps. I expect there to be similar effects in hotter stars. I am currently trying to get computer time from the NSF to complete the iron group elements including higher stages of ionization. Once the line data are complete, I will recompute the opacity tables for a range of abundances, then compute new grids of models, and synthesize spectra for comparison to observed spectra.

ATOMIC DATA SUMMARY
W.L. Wiese, NBS, Washington DC

Astronomers may obtain compilations of evaluated atomic data, as well as bibliographies of relevant literature references, from two principal sources (information and data material is usually freely supplied):

(a) The traditional source are the data centers of the National Bureau of Standards (NBS , USA, Address: Gaithersburg, MD. 20899), specifically the Data Center on Atomic Energy levels and Wavelengths (Director: W. Martin) and the Data Center on Atomic Transition Probabilities (Director: W. Wiese). Also, NBS operates a Molecular Spectroscopy Data Center (Director: F. Lovas).
   At the Joint Institute of Laboratory Astrophysics (JILA) Boulder, CO., an information center on Low Energy Atomic and Molecular Collision Data is operated (Director J. Gallagher).

(b) Due to worldwide data needs by the magnetic fusion research community, atomic spectroscopy data and especially data on atomic collisions (excitation, ionisation, charge transfer and recombination cross-sections and rates) are collected by the Center on Atomic Data for Controlled Fusion, Oak Ridge National Laboratories, USA; the Information Center at the Institute for Plasma Physics, University of Nagoya, Japan; the Japan Atomic Energy Research Institute, Tokai; and the Atomic Data Center, Queen's University, Belfast, Ireland. In addition, the International Atomic Energy Agency, Vienna, Austria publishes a quarterly Information Bulletin containing a comprehensive listing of current literature references on atomic data.

EFFECTS OF MOLECULAR LINE ABSORPTION ON STELLAR ATMOSPHERES
B. Gustafsson, Stockholm Observatory, Sweden

The general effects of molecular blanketing have been discussed in several reviews, see, e.g., Gustafsson and Olander (1979), Carbon (1979 and 1984) and Johnson (1986). Very schematically one finds that the line absorption generally causes a heating of the deeper layers (backwarming), while the upper layers may be cooled <u>or</u> heated. Cooling of the upper layers is in particular produced by absorption at wavelengths on the red side of the Planck maximum or, at shorter wavelengths, by absorption distributed through the atmosphere. Heating of the surface layers may result from absorption on the blue side of the Planck maximum, in particular if the absorption is concentrated towards the surface. An example of cooling molecular absorption is the absorption of CO VR lines in K stars, while the TiO line absorption heats the upper layers of M stars.

A number of facts should be noted:

(i) The surface effects are severely overestimated in LTE models if the lines in reality are formed in scattering instead of in absorption processes.

(ii) The collective effects of numerous individually very weak lines may well be of very great importance for the atmospheric structure - an example are the effects of "hot" combination bands of HCN on carbon-star atmospheres (Eriksson et al. 1984, Jørgensen et al. 1985).

(iii) There is an interesting coupling between the effects of a spherical extension

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of the atmosphere and the effects of molecular absorption (Watanabe and Kodaira 1978, 1979, Schmid-Burgk et al. 1981).

(iv) The picture outlined above changes qualitatively as a result of convective overshoot - in a realistic upper photosphere convection cools the gas (through adiabatic expansion) while radiation heats it (Nordlund 1985).

An interesting example of the complexity of the effects of molecular and metal-line absorption on the upper photospheric layers is the effects of line blanketing in the solar temperature-minimum region. Ayres (1981) and collaborators (Ayres and Testerman 1981, Ayres et al. 1985) have traced two components in the solar atmosphere, one hotter component visible in the Ca II H and K lines, and one cooler which shows up in the analysis of CO VR lines. Kneer (1983) has argued that two different equilibrium states might exist in classical model atmospheres; Nordlund (1985), however, finds that this is not the case if the metal lines are assumed to be formed in absorption. However, if the lines in the ultraviolet are assumed to be formed in scattering there are two different solutions to the model-atmosphere problem with very different surface temperature.

Two numerical methods for taking line blanketing into account are in current use - the Opacity Sampling (OS) method and the Opacity Distribution Function (ODF) method. The first-mentioned method is more flexible for individual models and easier to generalize to non-LTE cases and complex velocity fields, while the second method is more economical for the calculation of extensive grids of models. The two methods tend to give very similar results - for cool carbon stars, however, the ODF models deviate since the polyatomic opacity in the surface layers is not well correlated in wavelength with the absorption from diatomic molecules at greater depths (Ekberg et al. 1985). Similar problems are expected to occur for cool M stars where water vapour is an efficient absorber in the surface layers.

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IMPORTANT MOLECULAR DATA FOR THE ANALYSIS OF LATE-TYPE STELLAR SPECTRA

D.L. Lambert, Department of Astronomy, University of Texas

I have taken the point of view that a 15 minutes talk is not the forum for presenting lists of what we need from the community of physical chemists and chemical physicists, which anyhow is grossly underrepresented here so that pleas for more data, even specific pleas, are likely to be unheard.

Therefore, I shall just provide a few illustrations of what we need, and what

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is available, using as my basis two recent studies of CNO abundances of M, MS and S stars (Smith and Lambert 1985a and b) and of carbon stars (Lambert et al. 1986). The goal in these studies was to investigate how surface CNO-abundances change as asymptotic-giant-branch stars evolve and dredge up carbon from the helium-burning shell.

The molecular lines that are used in these studies are the CO V-R lines (for obtaining the carbon abundance in oxygen-rich stars and the oxygen abundance in carbon stars), OH V-R lines (for O-C in oxygen-rich stars), the C_2 Phillips and Ballik-Ramsay lines (for the C-O in carbon stars) and the Red CN system lines (for obtaining the nitrogen abundances). As extra checks we used the NH V-R lines for the nitrogen abundances and the CH V-R lines for C-O in carbon stars.

The basic need for physical data includes dissociation energies for observed molecules, and other molecules that are important in the molecular equilibria, and oscillator strengths - if LTE were not assumed one would also require a vast amount of collision cross-sections.

From this body of required data I select the following topics for discussion: the NH V-R frequencies, the f values for the CN Red system and the C_2 Phillips system, the f values for the OH V-R lines and the dissociation energy of CN.

The NH V-R lines were first detected in stellar spectra. The frequencies were obtained from rotational constants, derived from analyses of electronic systems, principally $A^3\Pi - X^3\Sigma^-$. Now, a few low V-R lines have been measured by tunable diode laser spectroscopy (Bernath and Amano, 1982). Fourier-transform spectra of the A-X system have also been obtained (Bernath, private communication) which has led to more accurate energy levels and reliable predictions of the frequencies of the V-R lines. This is important since the crowded spectra of late-type stars make precise frequencies necessary for a safe identification. Moreover, each transition is a triplet and the spacing is critical to the analysis of the strengths of saturated lines.

Recent experimental determinations of the CN $A^2\Pi$ lifetimes and studies based on solar observations tend to converge, although the reason for the departure of the Đuric et al. (1978) results for low v' values is still unknown. However, the POL-CI and the SCF+CI calculations of Cartwright and Hay (1982) and Lavendy et al. (1984), respectively, give significantly longer lifetimes, although the CASSCF calculations of Larson et al. (1983) agree much better with the experiments. The reason for the discrepancy between the calculations needs further investigation.

For the C_2 $A'\Pi$ state the experimental lifetimes are significantly longer that the calculated ones. The optimum stellar lines come from the $\Delta v=-2$ sequence and experiments for determining the relevant branching ratios would be of great help (cf. Lambert et al. 1986).

The OH V-R lines is a real success story, involving ab initio calculations, experimental measurements and the use of the Sun as a laboratory furnace. Grevesse et al. (1984) and Sauval et al. (1984) have shown that very consistent results with other oxygen abundance indicators are obtained with available physical data for the V-R and the pure rotational lines, provided that a realistic solar model is used.

The dissociation energy of CN is still unknown - recent determinations range from 7.5 to 8.0 eV. At determinations of nitrogen abundances in cool carbon stars an uncertainty of this magnitude is fatal since it leads to an uncertainty in the CN abundance of about 0.5 dex or more. Moreover, the N abundance as derived from the CN lines is proportional to the square of the CN abundance, due to the fact that most of the nitrogen is bound in N_2 molecules. Therefore, the uncertainty in D_0^o(CN) leads to an uncertainty of one order of magnitude in the nitrogen abundance.

In concluding, I would like to stress the importance of a continuous flow of information between stellar spectroscopists and physicists/chemists. We - the stellar spectroscopists - must make a strong effort to understand the methods of experimental molecular physics and theoretical quantum chemistry. How do we achieve this? We need a continuous education, through books, short courses, and meetings like the present one.

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4) MEETING: November 27th, 9.00

Non-Classical Problems, Non-Classical Atmospheres

Chairman: K. Kodaira

Topics were selected from an observational point of view to complement the theoretical sessions.

1. D. Gray presented a review on the progress in measuring macroturbulence in stellar atmospheres and its systematic dependence on the spectral type and the luminosity class of stars. He interpreted the systematic trend in terms of the convective activity in the outer envelope. Furthermore he reported on observations of curving of the bisector of absorption line profiles and of its variability, which required a new theoretical interpretation. Some basic questions were asked about the Fourier method used for the derivations of macroturbulence fields.

2. U. Heber discussed the results of NLTE fine analyses of spectra of 25 helium-poor hot subdwarfs. Their effective temperatures range from 25000 to 40000K. Helium is strongly underabundant, in some cases by more than a factor of 100. This is accompanied by large deficiencies of carbon and silicon in some stars. These peculiarities were explained by gravitational settling. As regards the evolutionary status of these stars, he concluded that they are extended horizontal branch stars with a very low envelope mass (less than 0.01 solar masses) and behave like helium main sequence stars. According to his view, the blue horizontal-branch stars observed in the globular cluster NGC6752 are the natural population-II counterpart to the field subdwarfs. During the discussion a question was raised about the different behavior of nitrogen relative to carbon. Heber answered that an extended low-rate mass-loss may play an important role in this concern.

3. D.M. Gibson was invited to discuss "Radio Aspects of Stellar Atmospheres". He pointed out the importance of radio data for determining macro-physical parameters such as mass-loss rates, structure of stellar coronae, and stellar activities. His HR diagram, showing the distribution of radio-loud stars, called a debate how far this is affected by selection effects.

4. K. Koyama demonstrated how we can understand the X-ray bursts under the assumption that the peak luminosity reaches the Eddington limit in a consistent manner with the current picture of neutron stars. The decay phase of the X-ray bursts can well be interpreted with a scattering atmosphere dominated by Compton processes. The high red-shift of the Fe absorption line detected by the Temma satellite was accounted for by the high surface gravity of a neutron star. This self-consistent picture led to a claim that the distance to the galactic center should be 6-7kpc. This last point, however, was questioned by some attendants.

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5) MEETING: November 27th, 11.45 - 12.30

Miscellaneous scientific papers

Chairman: B. Gustafsson

1. R.K. Prinja reported on a study on narrow absorption components and variability in UV P Cygni profiles of early-type stars (together with I.D. Howarth). An extensive set of velocity and column density measurements of both narrow absorption components and 'underlying' P Cygni profiles have been obtained for a sample of 21 main sequence, giant, and supergiant stars with spectral types B1 to O4. To study variability characteristics every unsaturated resonance line doublet profile was modelled in each of 322 uniformly extracted high resolution IUE spectra. Mass-loss rates are given for 19 stars. Variability in $\dot{M}$ is usually at the 10% level, on timescales of a day or longer; changes of a factor of 2 or greater are not observed. Narrow components were observed at least some of the time in every star with unsaturated P Cygni profiles. In many cases Copernicus observations taken a decade earlier show features at the same velocities. Multiple components (up to 3) are not uncommon. Central velocities and velocity dispersions average 0.8 and 0.06 of the terminal velocity respectively, while column densities are typically ~ 14.5 dex cm^{-2}, and show substantial (>2X) variability in most stars. This variability appears to be unrelated to changes in the underlying profiles. A search for correlations between different aspects of our data reveal few systematic trends, but there is a suggestion that rapid rotators may be exceptional in some respects.

2. Underhill reported on the ongoing analysis of Wolf-Rayet spectra which she and A.K. Bhatia (Goddard Space Flight Center) are carrying out. The results indicate that Wolf-Rayet stars are like B1 to O9 stars except that they have conspicuous, hot mantles. In WC stars the electron temperature in the mantle is between 5×10^4 and 10^5 K; in WN stars it is greater than 10^5 K. The composition of Wolf-Rayet atmospheres is normal (solar), just as for OB stars.

3. R. Wehrse summarized recent work on white dwarf atmospheres, as a complement to his contribution in the Com. 36 Reports on Astronomy, IAU Trans. XIXA.

The meeting ended in a general discussion of the need, and the adequate form for the Reports on Astronomy.

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