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Theoretical and Experimental Studies in Ultraviolet Solar Physics

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I. INTRODUCTION

In Section II of this Semiannual Status Report we describe the results of our research on the processes and parameters in atomic and molecular physics that are important to solar physics. In general our research program covers three categories of study:

(1) The measurement of atomic and molecular parameters that contribute to discrete and continuous sources of opacity and to abundance determinations in the sun.

(2) The line broadening and scattering phenomena that must be understood to interpret solar spectral features.

(3) The development of an ion-beam spectroscopic source which will be used for the first measurements of electron excitation cross sections of transition region and coronal ions that have specific importance in solar electron density and temperature determinations.

Changes in instrumentation and new approaches that will be used in future related work are described in Section III.

In Section IV we have listed the papers published during this period. These papers report the measurement of atomic and molecular parameters that contribute to discrete and continuous sources of opacity and to abundance determinations in the sun and to line broadening phenomena that must be understood to interpret solar spectral features.

II. SPECTROSCOPIC RESULTS

II-A. Photoionization Cross Section Measurements with the Windowless Shock Tube

The newly constructed EUV shock tube facility at this laboratory has been used to measure, absolutely, the photoionization cross section of atomic hydrogen (Palenius, Kohl and Parkinson 1975, in press). The agreement between the observed and the theoretical values demonstrates the capability of the apparatus for making absolute photoabsorption measurements with uncertainties in the ±10 - ±20% range. Our program to measure the absolute photoionization cross sections of O I, C I, and N I will continue after some further improvements of the apparatus.

The measured values are collected in Fig. 1 where the absolute photoionization cross section of atomic hydrogen (in Mb) is plotted versus wavelength. The observed data points for five different shocks are plotted for 17 different wavelengths and the average values of each wavelength are indicated by the solid circle and bar. The curve represents the theoretical values and the dotted lines mark ±20% excursions from the theoretical curve. Almost all observations are within 20% and the average points are in closer agreement with theory and fall within the expected experimental uncertainties. The observed average values are given in Table I together with the theoretical values that were calculated from the theoretical expression given by Ditchburn and Öpik and the

Gaunt factors tabulated by Karzas and Latter.

Our data show a small tendency to be systematically higher than the theoretical values for wavelengths shorter than about 750 Å. Because additional photon loss could be due to Rayleigh scattering from the many Ne atoms, the cross section for this scattering was calculated by Dr. G. Victor. The semiempirical calculations used the available data for the ground state f-values and for the continuum photoionization cross section of Ne I. However, the calculated cross section for Rayleigh scattering was found to change our measured cross section by only about 1% for $\lambda < 750$ Å. There is also a very small tendency towards a systematic discrepancy between observation and theory for wavelengths around 850 Å. This region corresponds in wavelength to the location of the hydrogen atom-atom radiative recombination continuum. The FUV shock emission has been found to give a weak continuum for $\lambda \lesssim 915$ Å, which could be measured only with much wider spectrograph slits than were used for the absorption measurements. The measured emission around $\lambda 850$ Å was found to be larger than that at higher and lower wavelengths. From a limited amount of data it appears likely that the shock emission would explain the systematic discrepancy around $\lambda 850$ Å between our measurements and theory. No compensation for these absorption and emission effects has been made in the presented results.

Since future work will rely on the H I measurements as a demonstration of the reliability of the apparatus, it was important to make a thorough error analysis. This required some additional measurements.

There is substantial evidence that the shock-heated gas behind the reflected shock front during the temperature and pressure plateau was in a state of LTE. The uncertainty in the atomic hydrogen number density determination was, therefore, mainly due to the 2% error in the temperature measurement, the 4% uncertainty in the pressure measurement, and the 1% uncertainty in the initial gas mixture concentrations. From these errors and from the fact that the electron number density calculated with the chemical equilibrium program agreed to within 5% with the measured electron number density, we estimate a most probable error in the hydrogen number density determination of about $\pm$ 5%.

The uncertainties of the reproducibility of the flashlamp (5%), the calibration of the mesh filters (0.5%), the photometric reduction (8%) and the normalization of the shock spectra to I_0 for $\lambda > 920$ Å (2%) gave a most probable error in the I/I_0 determination of about $\pm$10%.

Assuming independent errors, we find a most probable error in the H I photoionization cross section for the data of each shock of 10, 12, and 15% for measurements near the wavelengths of 900, 750, and 600 Å respectively. The dependence on wavelength is due to a systematic tendency to have more absorption for the higher wavelengths. The random errors for the average data points of the 5 shocks would be reduced by a factor of 0.45.

In addition to the above errors, there were systematic errors. The errors due to the gas flow out of the openings in the shock tube should be less than 4% and those due to boundary layers less than 2%. These two effects are to some extent compensated by the observed shock emission. The effect of this was found to vary with wavelengths from about 5% at the series limit to a maximum of about 10% at 850 Å and then rapidly decrease with wavelength, becoming less than 2% at 800 Å. No compensation for these absorption and emission effects has been made to the results presented here.

An overall estimate was made of the uncertainties in the averaged absolute determinations of the cross section. These are: about $\pm 7\%$ for wavelengths near the series limit, +6 to −15% from about $\lambda 850$ Å down to about $\lambda 750$ Å, and then for shorter wavelengths +12 to −7%. Treating the theoretical curve as a standard, we give the percent standard error in Table I. Most of the measured average values for $\lambda > 712$ Å fall within the expected uncertainty limits. However, the values for $\lambda < 712$ Å have somewhat larger discrepancies than expected.

II-B. f-Value Measurements

II-B-1. Alkaline-Earth Metal Group f-Values

The hook-method has been used by Parkinson, Reeves and Tomkins to measure the following lines in Ca I: $4s^2\ ^1S_o$ - $4snp\ ^1P_1^o$ (n = 4-17) $4s^2\ ^1S_o$ - $3d4p\ ^1D_1$, in Sr I: $5s^2\ ^1S_o$ - $5snp\ ^1P_1^o$ (n = 5-26) $5s^2\ ^1S_o$ - $4d5p\ ^1P_1^o$, $4d5p\ ^3P_1^o$, $5s5p\ ^3P_1^o$ and in Ba I: $6s^2\ ^1S_o$ - $6snp\ ^1P_1^o$ (n = 6, 7 and 12-20) $6s^2\ ^1S_o$ - $5d8p\ ^3P_1^o$, $5d8p\ ^3D_1^o$ and $5d4f\ ^1P_1^o$. In addition a value of the photoionization cross section at threshold has been obtained for Mg I, Ca I and Sr I by plotting the gf-values of lines in the principal series according to the quantum defect method. For Mg I, we have used the gf-values measured earlier by Mitchell (1975) also with the hook techniques. Extrapolation of the bound state gf-values for Mg I yield 2.36 Mb at threshold in agreement with the calculations by Dubau and Wells (1973) and larger by a factor of 2 than the measurements of Ditchburn and Marr (1953) based on vapor pressures. For Ca I, extrapolation of our measured bound state gf-values yield 2.75 Mb at threshold which is larger by a factor of 2.2 than earlier data of Hudson and Kieffer (1971) based on vapor pressures. Our recommended factor to correct the previously published values agrees with the suggested revised scale of McIlrath and Sandeman (1972) for absolute absorption cross sections of Ca I at 1886.5 and 1765.1 Å. For Sr I, extrapolation of our bound state gf-values yield 11.2 nb at threshold which is larger by a factor of 1.9 than the data of Hudson, Carter and Young (1969) again based on vapor pressures.

A paper describing this work on the alkaline earth metal spectra is now in preparation.

II-B-2. Iron Group f-Values

a. Sc I

The final data reduction on the Sc I gf-values is nearing completion. Dr. G. Bell of Harvey Mudd College has measured the absolute gf-values for the resonance lines of Sc I near 400 nm. These are the best gf-values available and will be used to place on an absolute scale, the relative gf-values of 100 transitions in the Sc I spectrum between 644.8 nm and 199.9 nm which we have measured by the hook method. Earlier beam-foil method measurements of the life-time of the $^2F^o_{3/2}$ and the $^2D^o_{3/2}$ states yield gf-values for the resonance lines that are too small by a factor of 1.5.

b. Ti I

The analysis by Dr. P.L. Smith of the Ti I data for 320 nm $\leq \lambda \leq$ 600 nm is nearing completion. Additional data for 180.0 $\leq \lambda \leq$ 3200 nm will be obtained when study of the photoionization cross section of Ti is resumed.

c. Cr I

Measurements of wavelengths, absorption cross sections and oscillator strengths have been made and reported by Huber, Sandeman and Tubbs (1975) for the spectrum of Cr I between 179.8 and 200 nm. The absorption spectrum of the Cr vapor was recorded photoelectrically and by photography. By use of the hook method the column density of neutral Cr atoms in the ground state was determined with the aid of the accurately known oscillator strengths of the resonance lines near 427 nm. The absorption cross section of the autoionized lines that dominate the ionization continuum were placed on the absolute scale in this manner. The wavelengths of many hitherto unreported lines were measured near the ionization limit and a new value for the ionization potential of 54575.6 $\pm$ .3cm^{-1} was determined.

In conjunction with these measurements Huber and Sandeman have measured the gf-values of 148 transitions in the Cr I spectrum with wavelengths between 200 and 541 nm. The hook and absorption methods for strong and weak lines respectively were used. Of these gf-values, 114 of them have been measured for the first time. This work is now in preparation for publication.

d. Ni I

Extension measurements using the hook method have been made by Huber and Sandeman of the gf-values of the lines in the Ni I spectrum. Approximately 250 transitions have been studied between 196 nm and 397 nm. The analysis and data reduction will continue on these gf-values.

II-B-3. f-Values for the Second Spectra of the Iron Group

The discussion of the correction to the gf-value data of Warner (1967) is being prepared by Smith for publication. The semiempirical f-values of Kurucz and Peytremann (1975) will be included in the comparison in order to provide an assessment of the usefulness of this large body of data also.

II-C. Refractive Index Measurements

One of the shortcomings of current theoretical, line-blanketed, solar models (Kurucz 1974a, 1974b) is the omission of line strengths of diatomic molecules. This omission is a result of the scarcity of data for these molecules, especially for those such as C_2, CN, CH, NH and OH which are present in the sun (Mount et al., 1972).

In order to remedy this situation, the Theoretical Group of the Atomic and Molecular Physics Division of the Center for Astrophysics is planning to develop new calculational techniques for the study of simple diatomic molecules. One measured property of gases that can be used to assess such calculations is the refractive index, especially in the vacuum ultraviolet wavelength region. In an effort to determine whether our laboratory apparatus could be used to make refractivity measurements of sufficient accuracy to be useful in evaluations of the new calculation techniques, measurements of the refractive index of He, H_2, O_2, CO, Kr, (Smith, Huber and Parkinson) and air (Smith and Parkinson) were made for approximately $1700\ \text{Å} \leq \lambda \leq 2900\ \text{Å}$. The feasibility of this type measurement has been demonstrated and the results are being prepared for publication. It is hoped that these measurements can be extended to lower wavelengths and to gases such as N_2 and NO which are also of interest in the assessment of the theoretical methods.

II-D. Piston Compressor

II-D-1. Line Broadening

Dr. Driver and Dr. Snider carried out an experiment with the piston compressor to study the mechanism of neutral line broadening for the calcium 422.7 nm resonance line broadened by a high temperature helium gas. The experimental setup is similar to that used by Eckart (1975) for the Na D broadening. Hot helium was produced in the piston compressor in a temperature range of 3000 - 6500 K and a density range 2 - 6 x 10^{20} cm^{-3}. The calcium was present in the compressor as an impurity. The calcium line shapes were measured in absorption using a twelve channel polychromator detection system. The helium pressure, number density and the Boltzmann temperature of the calcium atoms were measured separately. Because of the low electron density in the compressor it was found that the Boltzmann temperature did not coincide with the helium kinetic temperature. This confirmed similar findings by Eckart in his study of the Na D line broadening.

Our measured result at a temperature of 4500 K is

$$\frac{\gamma}{n} = (42.0 \pm 3.5) \times 10^{-22}\ \text{Å}\ cm^{-3} \quad .$$

The temperature dependence of $\frac{\gamma}{n}$ does not match any of the similar theories of neutral line broadening such as the Van der Waal theory or the Lennard-Jones interatomic potential theory (Hindmarsh, *et al*, 1967).

II-D-2. Radiation Redistribution

The laser scattering experiment on the piston compressor is continuing. Work has been going on to enable the flashlamp pumped dye laser to "lase" at two different wavelengths. This would allow us to monitor the scattering contribution from dust particles in the compressor and thus separate out true fluorescence from this spurious source of scattering.

II-E. Series Spectra

The analysis of the spectrum of laser excited barium is now almost complete and the results are being prepared for publication by Dr. C. Skinner.

Thirty-four new emission lines arising from the non-linear interaction of the laser with barium atoms have been observed and identified. These lines are due to parametric four wave mixing processes. Four additional lines were seen which had been observed previously, as reported in Semi-Annual Report No. 20. The total of thirty-eight form a complete and consistent picture of all the most likely four wave processes possible in this system. This work is allied to the technique of generating intense tunable VUV radiation by frequency mixing which is of considerable interest in the extension of laser spectroscopy to the VUV region important in solar physics.

II-F. Flash Pyrolysis

The flash pyrolysis technique has been used by R. Roig in his study of three spectra.

a. Ba II

The spectrum of singly ionized barium (Ba II) has been extended. Fifteen new levels have been established and 24 new lines have been observed. Photoionization has been shown to be the dominant ionization mechanism in the flash pyrolysis technique. A paper on the extension to the Ba II spectrum has been published by Roig and Tondello (1975).

b. Al I

The classification of the $3s3p(^3P)np$ states of Al I, as seen in absorption from the ground state of the atom was also completed. The relative photoionization cross-section was measured in the region $200.0 \text{ nm} \geq \lambda \geq 110.0 \text{ nm}$. By using the absolute measurements of Kohl and Parkinson (1973), the results could be put on an absolute scale. The astrophysically important transitions to the $3s3p^2\ ^2S$ autoionizing state were remeasured for their Fano/Shore parameters and for their wavelengths. Agreement was obtained with the results of Kohl and Parkinson (1973) for widths and peak cross sections. However, the asymmetry parameter was found to be positive and of the same magnitude as previously measured. The ab initio calculations of Le Dourneuf et al. (1975) show excellent agreement with the present measurements of the autoionizing parameters. This data has been submitted for publication and is now available in preprint form.

c. B I

Work has begun on the classification of the neutral boron, B I, spectrum. In the preliminary experiments, transitions to the $3s3p(^3P)np$ states have been viewed in absorption from both the $3s^2 3p\ ^2P$ ground state and the metastable $3s3p^2\ ^4P$ state. If the series are sufficiently unperturbed, it is hoped that the interval between these states can be determined. Present estimates have been determined solely by the use of isoelectronic sequences (Edlén et al., 1969). It is also hoped that the relative photoionization cross section could be measured in the region 150.0 nm $\geq \lambda \geq$ 135.0 nm.

III. TECHNIQUES AND INSTRUMENTATION

III-A. The Ion-Beam Apparatus

Dr. J.L. Kohl has continued to build the ion-beam apparatus, which will be used to measure electron excitation cross sections and other basic parameters of multiply charged ions.

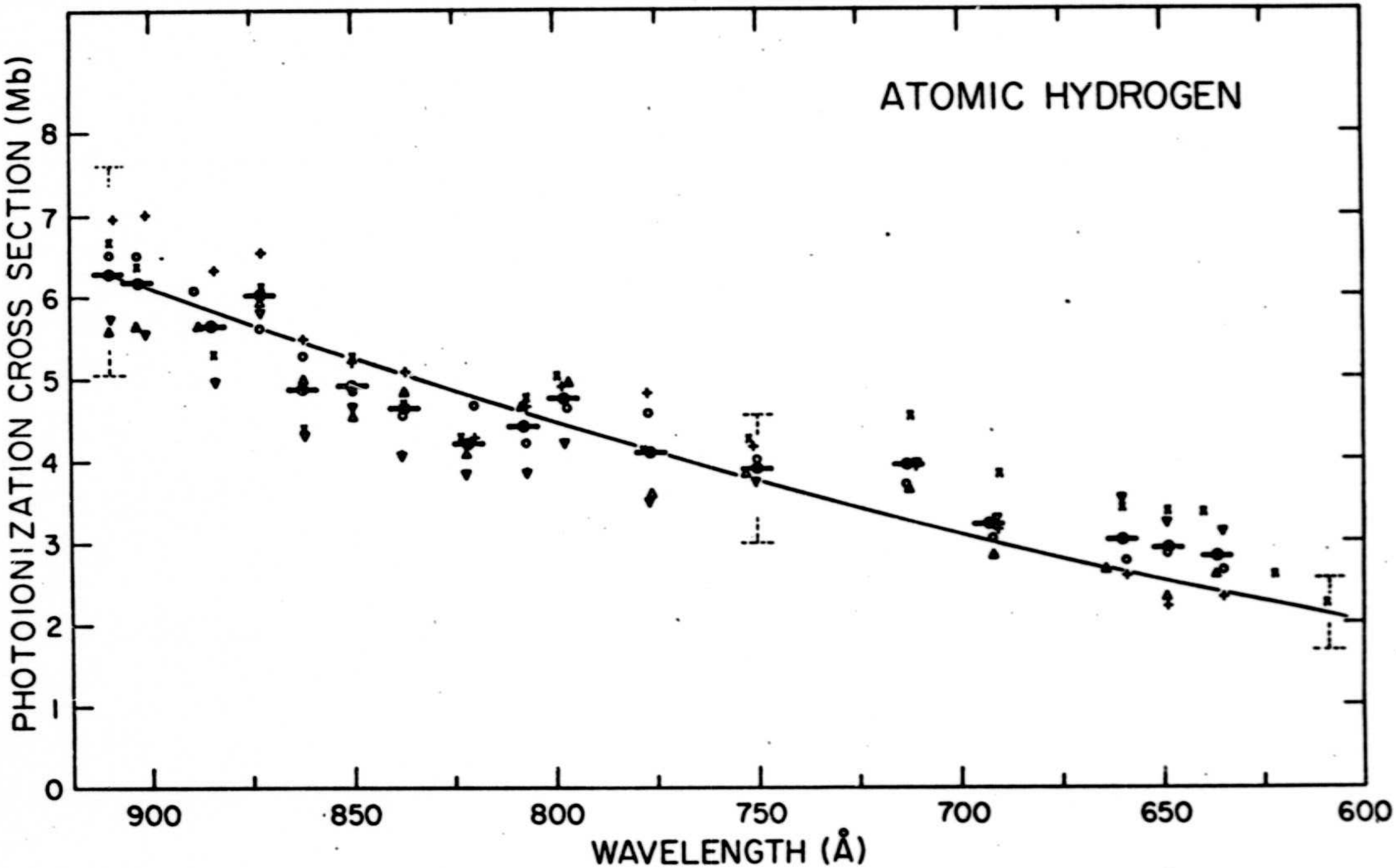
During this grant period we completed the construction assembly and performance tests of the vacuum systems that maintain a high vacuum environment for the ion source in the region between the pole faces of the electromagnet that is used to select the mass to charge ratio of the ion beam. We have also conducted performance tests and evaluations of the oscillatory discharge ion source. During the past few weeks we have succeeded in operating the discharge of the ion source at a current of 7 amps and a discharge voltage of 300 volts. The discharge appears to be well behaved over short periods of time and we are presently making a few minor modifications to the apparatus that will make it possible to run the discharge for extended periods of time. We have extracted a 10 mA current of ionized nitrogen from the source. We have also begun to design the beam optics that are needed to extract the ions from the ion source, analyze them for their charge to mass ratio, extract them from the magnetic field and focus them into the required beam shape.

This project is partially supported by the Smithsonian Institution.

III-B. Vacuum Mach-Zehnder Interferometer

The design of a new light source facility to be used with the interferometer is underway.

In addition the Muffoletto Optical Company has obtained several 3" single crystals of MgF_2 and CaF_2 and is attempting to produce beam splitters, compensation plates and furnace windows of the quality required for interferometry in the wavelength region of the ionization limits of the astrophysically important iron group elements.



ATOMIC HYDROGEN
PHOTOIONIZATION CROSS SECTION (Mb)
0
1
2
3
4
5
6
7
8
900
850
800
750
700
650
600
WAVELENGTH (Å)

Figure 1

Table I

Comparison of Measurements and Theory

λ(Å)	$\sigma_{Exp.}$ (Mb)	$\sigma_{Theor.}$ (Mb)	$\sigma_{Exp.} - \sigma_{Theor.}$ (Mb)	% Standard error from theory
911.753	(6.28)[a]	6.31	-(0.03)	(<1)
910	6.25	6.28	-0.03	<1
903	6.16	2.15	0.01	<1
885	5.62	5.83	-0.21	-4
872	5.98	5.61	0.37	7
862	4.85	5.44	-0.59	-11
850	4.83	5.24	-0.41	- 8
838	4.60	5.05	-0.45	- 9
822	4.19	4.79	-0.60	-13
808	4.40	4.58	-0.18	- 4
798	4.73	4.42	0.31	7
777	4.09	4.12	-0.03	- 1
752	3.89	3.79	0.10	3
712	3.93	3.25	0.68	21
691	3.22	3.00	0.22	7
660	2.99	2.64	0.35	13
649	2.82	2.53	0.29	11
636	2.81	2.39	0.42	18
623	2.57	2.25	0.32	14
609	2.23	2.12	0.11	5
			average 0.03	

[a] Extrapolated value.

IV. PUBLICATIONS

"The Spectrum of Cr I between 179.8 and 200 nm Wavelengths, Absorption Cross Sections and Oscillator Strengths".
M.C.E. Huber, R.J. Sandeman and E.F. Tubbs
Proc. R. Soc. Lond. A342, 431-438, 1975.

"The Shape of the Sodium D Lines in a High-Temperature Helium Atmosphere".
M.J. Eckart
J. Phys. B., 8, #6, 852-863, 1975.

"Extensions to the Spectrum of Singly Ionized Barium (Ba II)".
Randy A. Roig and Giuseppe Tondello
JOSA 65, 829, 1975.

"The Refractive Index of Krypton for 168 nm $\leq \lambda \leq$ 288 nm".
Peter L. Smith, W.H. Parkinson and M.C.E. Huber
To be published in Optics Communications.

"Absorption Spectrum of Laser-Populated ^3D Metastable Levels in Barium".
J.L. Carlsten, T.J. McIlrath and W.H. Parkinson.
J. Phys. B.: Atom. Molec. Phys. 8, 38-51, 1975.

"Photoionization of Barium Clouds via the ^3D Metastable Levels".
J.L. Carlsten
Planetary and Space Science 23, #1, 53-59, 1975.

"Stimulated Stokes Emission with a Dye Laser: Intense Tuneable Radiation in the Infrared".
J.L. Carlsten and P.C. Dunn
Optics Communications 14, #1, 8-12, 1975.

REFERENCES

Ditchburn, R.W. and Marr, G.V. 1953, Proc. Phys. Soc. A66, 655-6.

Ditchburn, R.W. and Opik, U. in Atomic and Molecular Processes edited by D.R. Bates (Academic Press, New York, 1962).

Le Dourneuf, M., Lan V. Ky, Burke, P.G. and Taylor, K.T. 1975, Preprint.

Dubau, J. and Wells, J. 1973, J. Phys. B: Atom. Molec. Phys. 6, L31-3.

Eckart, M.J. 1975, J. Phys. B., Atom. Molec. Phys. 8, 852-863.

Edlén, B., Palenius, H.P., Bockasten, K., Hallin, R., and Bromander, J. 1969, Solar Phys. 9, 432.

Hindmarsh, W.R., Petfand, A.D. and Smith, G. 1967, Proc. R. Soc. A 297, 296.

Hudson, R.D. and Kieffer, L.J. 1971, Atómic Data 2, No. 3 205-62.

Hudson, R.D., Carter, V.L. and Young, P.A. 1969, Phys. Rev. 180, 77.

Karzas, W.J. and Latter, R. 1961, Ap.J. Suppl. Ser. 6, 167.

Kohl, J.L. and Parkinson, W.H. 1973, Ap.J. 184, 641.

Kurucz, R.L. 1974a, Solar Physics, 34, 17.

Kurucz, R.L. 1974b, Astrophys. J., 188, L21.

Kurucz, R.L. and Peytremann, E. 1975, A Table of Semiempirical gf Values, Smithsonian Astrophysical Observatory Special Report #362. Smithsonian Institution Astrophysical Observatory. Cambridge, Mass. 02138.

McIlrath, T.J. and Sandeman, R.J. 1972, J. Phys. B: Atom. Molec. Phys. 5, L217-19.

Mitchell, C.J. 1975, J. Phys. B: Atom. Molec. Phys. 8, 25-9.

Mount, G.H., Linsky, J.L., and Shine, R.A. 1972, Solar Physics, 26, 42.

Warner, B. 1967, Mem. Roy. Astr. Soc. 70, 165.