U. Calif

Status Report on NASA Grant

NGR-05-007-046

Studies of the Solar System and Probable Lunar Abundances of Elements of Geochemical and Metallurgical Significance

INTRODUCTION

It has often been postulated that the moon is composed of non-volatile material whose chemical composition can be identified with that of the primordial solar system. Recent advances in geochemistry and cosmochemistry suggest that the chondritic meteorites, often chosen as samples of the non-volatile constituents of the original solar system, have been strongly affected by fractionation processes. Thus it seems likely that the only tractable sample of the primordial solar system composition is the sun itself-Urey noted that the density of the moon could be explained in terms of non-volatile material of solar composition, whilst a moon of chondritic composition would have too high a density Furthermore, a "chondritic" moon would contain so much radioactive material that it would generate a great deal of heat. Consequently, the interior of the moon would be mostly melted and the body would have no rigidity in contradiction to the observational evidence as discussed by MacDonald. Likewise, the interior of Mars would have melted, the metals would have settled to the core, and the planet should show a density distribution more nearly similar to that of the earth, rather than to a homogeneous body as it actually does.

Therefore we regarded it highly probable that the moon is composed of undifferentiated, non-volatile material of essentially solar composition, and undertook the determination of more accurate abundances of certain elements in the sun.

(HC) $2.00
(MF) .50

Our observational data consists of high resolution spectrum tracings obtained in collaboration with Director Orren Mohler of the McMath-Hulbert (solar) Observatory of the University of Michigan, and some high resolution tracings obtained by Professor Walter Mitchell (Ohio State University) with the Snow solar telescope at Mount Wilson Observatory.. Many of these tracings were obtained with a monochromator to eliminate scattered light so that accurate line shapes could be obtained. In some instances it was possible to measure the line profile at several points on the solar disk and thus obtain checks on the model atmosphere employed.

We are considering several of the more important, abundant elements and their ions, and in addition several of the less abundant elements, viz SbI, BaII, BeI, CdI, NbI, NbII, GaI, GeI, AuI, InI, MoI, RuI, AgI, YbI, YI, YII, ZrI, and ZrII.

The abundant elements and the rare elements pose different problems.

Consider first the abundant elements. Mugglestone and O'Mara (1) showed that line broadening and, in particular, stark broadening can play an important role in the determination of the abundances of elements in the sun; they used sodium at their example. In our project, O'Mara is carrying out a similar investigation for other light elements and in addition for the important elements, iron and titanium. He constructed two model atmospheres which he believed would bound that true solar model. One of the models was constructed by extrapolating the Pierce-Waddell (2) temperature distribution, based on limb-darkening at 5000A, into the upper photospheric region. This temperature distribution is believed to be a lower bound to the temperature distribution

in the upper layers. The other model was constructed by joining up the temperature distribution given by Pagel (3) for the low chromosphere with that obtained from the Pierce-Waddell limb darkening curves at 9000A, while in the deeper layers the temperature distribution obtained from limb darkening curves at 16,500A° (where the opacity is lowest) is used. In view of the recent work of Noyes et al (4) this temperature distribution should represent an upper bound on the temperature in the upper layers. A difficulty in integrating the equation of hydrostatic equilibrium arises in choosing the starting values of the gas pressure. This problem can be overcome to some extent by adjusting the starting value of the gas pressure so that values of $d\tau_\lambda/dT$, computed from the model atmosphere agree with those gotten from the limb darkening data.

In their investigations, Mugglestone and O'Mara (1) Goldberg, Müller and Aller (12), and Aller, O'Mara, and Little (13) employed a weighting function method which is not suitable when one wishes to use a damping constant that varies with the depth. We have discarded this method in favor of the direct computation of the line profiles. O'Mara has prepared a computer program that computes line profiles in a form that can be fitted directly to the double-band-pass observations of Mohler and Mitchell (5). He computes the Stark damping constants from the tables of Griem (6), while the van der Waals' damping constants are computed from the Lindholm Foley theory (as described for example by Aller [7]). He has taken the damping constants for iron and titanium from the experiments of Kusch (8) and Meyer (9).

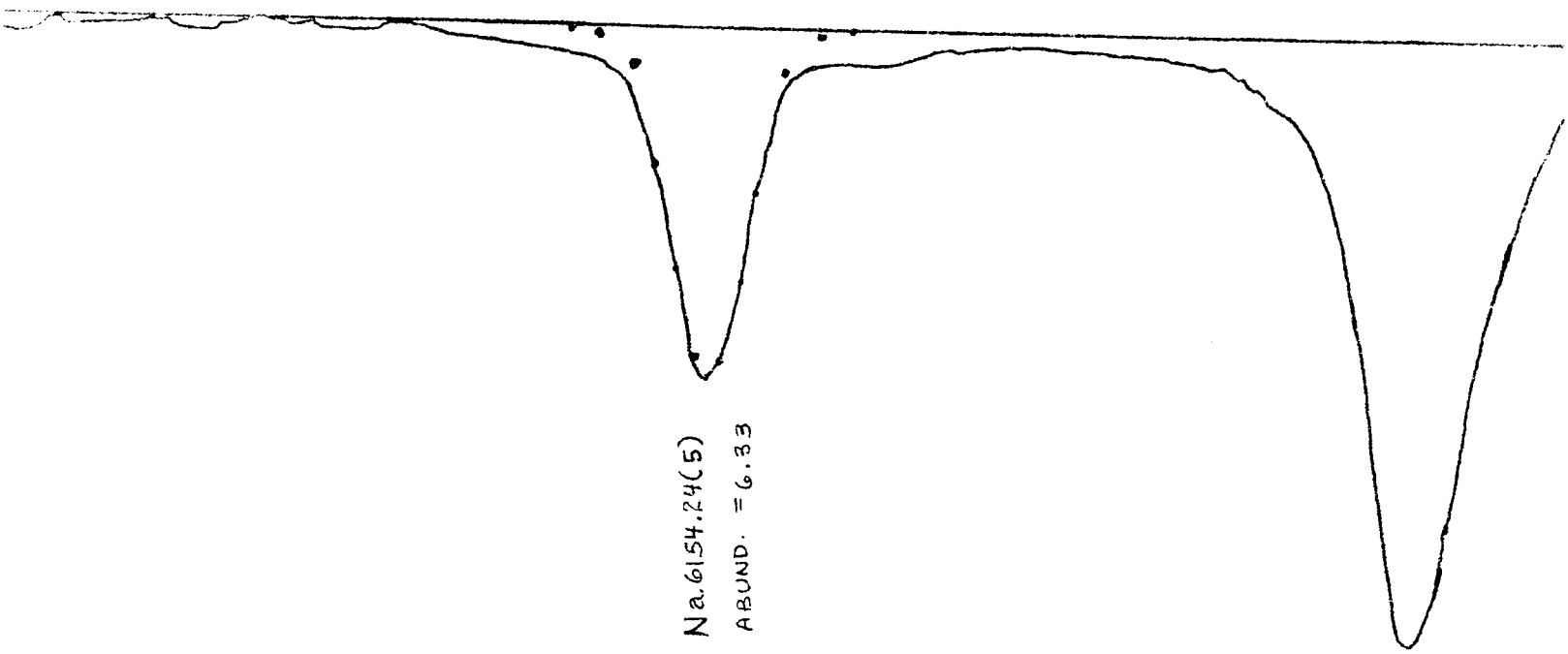
O'Mara's preliminary results indicate that the Lindholm-Foley theory gives van der Waals damping constants that are too small, a result similar to that found by Weidemann (10). Furthermore, O'Mara

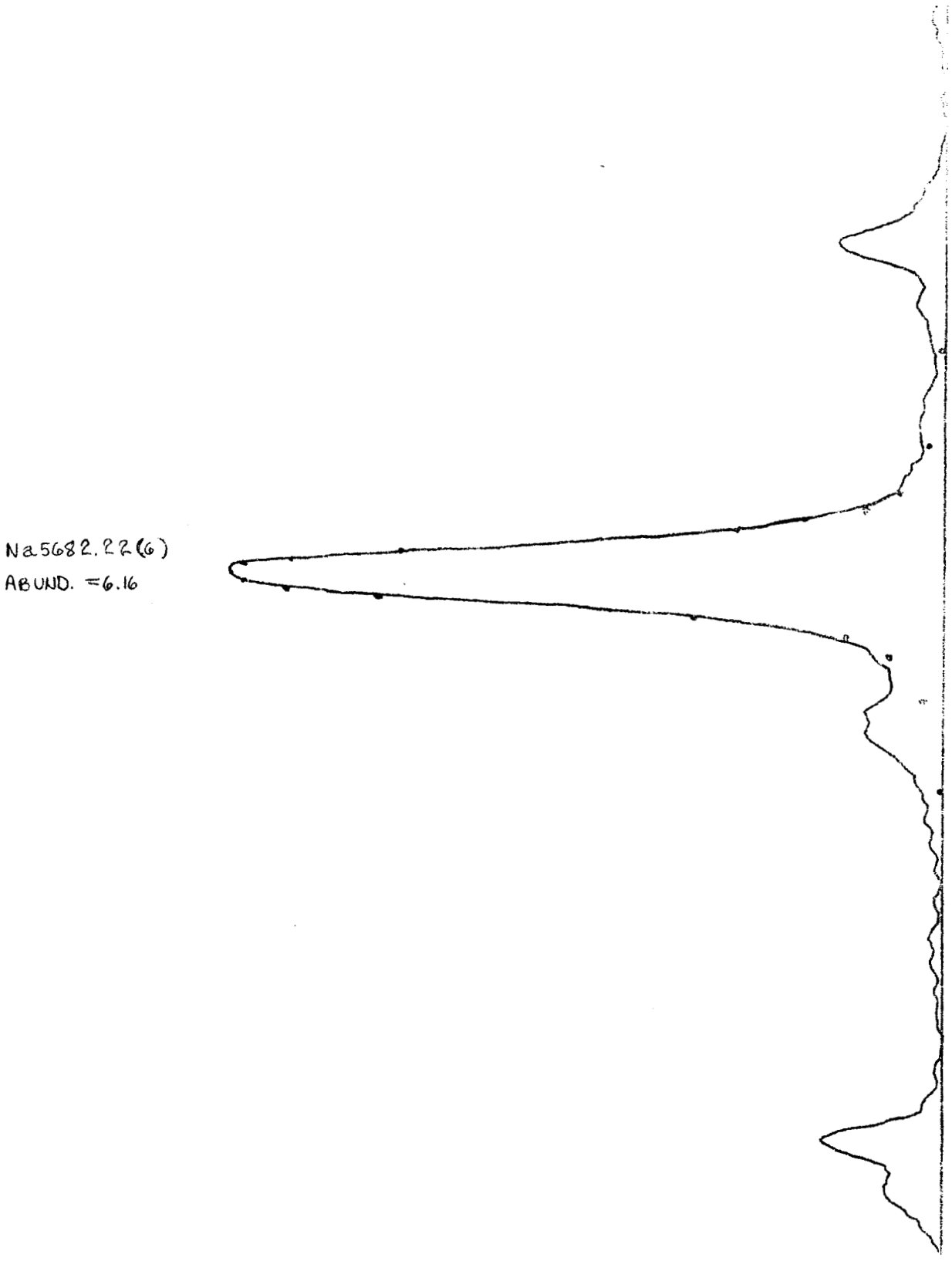
finds that the breadth of the carbon lines in the visible region cannot be explained by the aforementioned mechanisms: more likely this anomalous broadening is produced by the formation of quasi-molecules of C2. This phenomenon, discovered in laboratory spectra, has been described for example by Ch'en and Takeo (11). It seems unlikely, however, that the present abundance determinations will drastically alter the abundances established by Goldberg, Müller and Aller (12).

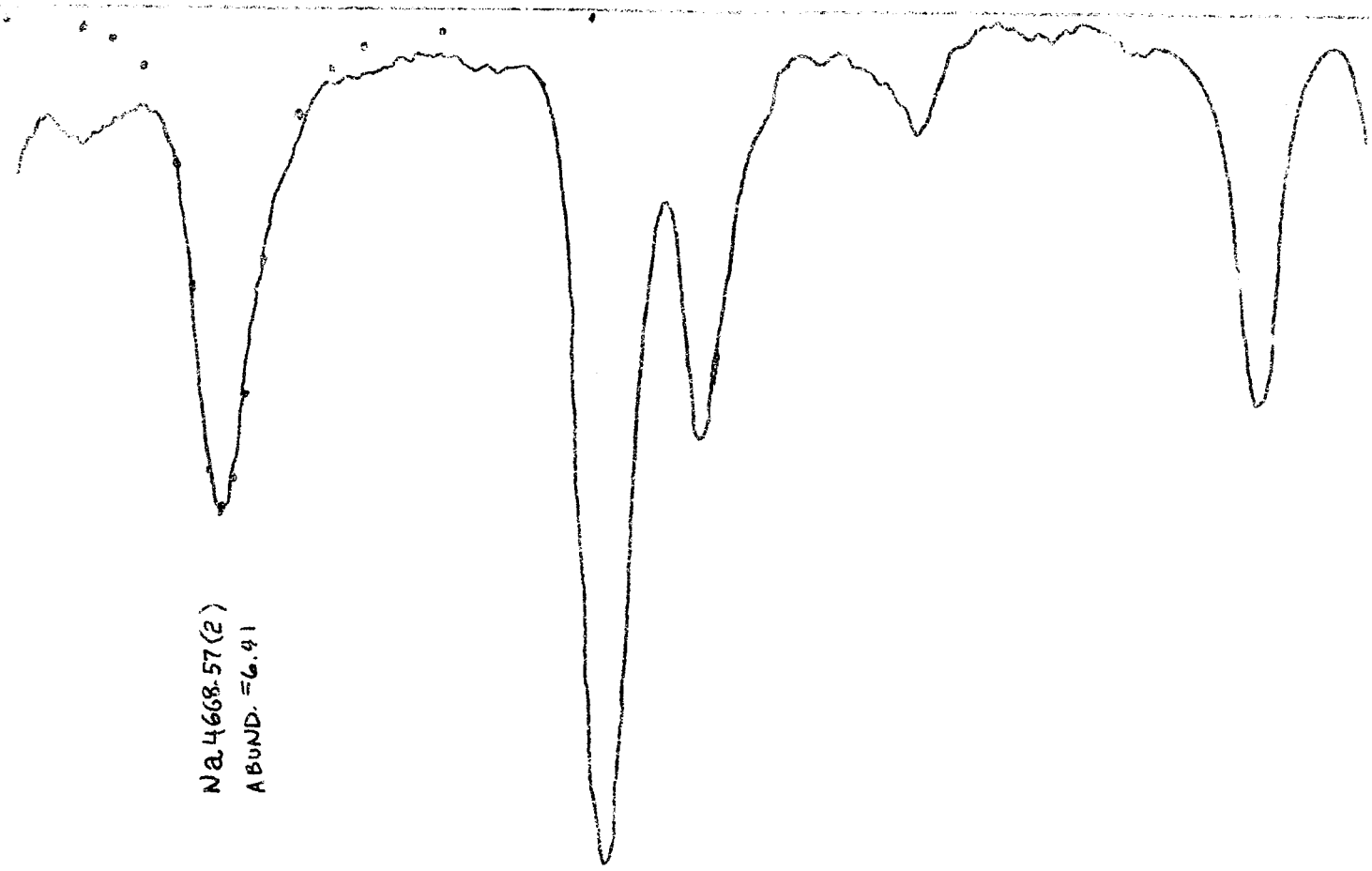
In yet another way, the problem of spectral line formation is difficult. In an enclosure and under most conditions in a stellar atmosphere, a single pair of parameters, namely the temperature and the electron or ion density, can be used to characterise the populations of all atomic and ionic levels. In the upper layers of the solar atmosphere no such simple situation holds and one must evaluate corrections to the calculations made by the simple LTE or local thermodynamic equilibrium theory. Some workers obtained very large corrections, contending that the abundances derived from the LTE assumption for elements such as Ti or Fe could be in error by a factor of eight or ten. Work carried out more recently by a number of investigators indicates that while such deviations exist, they are more likely to be of the order of 10-30 percent, rather than factors of five or ten. Thus, for sodium, O'Mara finds that by a combination of improved model atmospheres, more sophisticated line broadening theories, and deviations from LTE, the spectral lines of sodium, which previously gave discordant results, now give accordant conclusions and a sodium abundance in which we can have confidence.

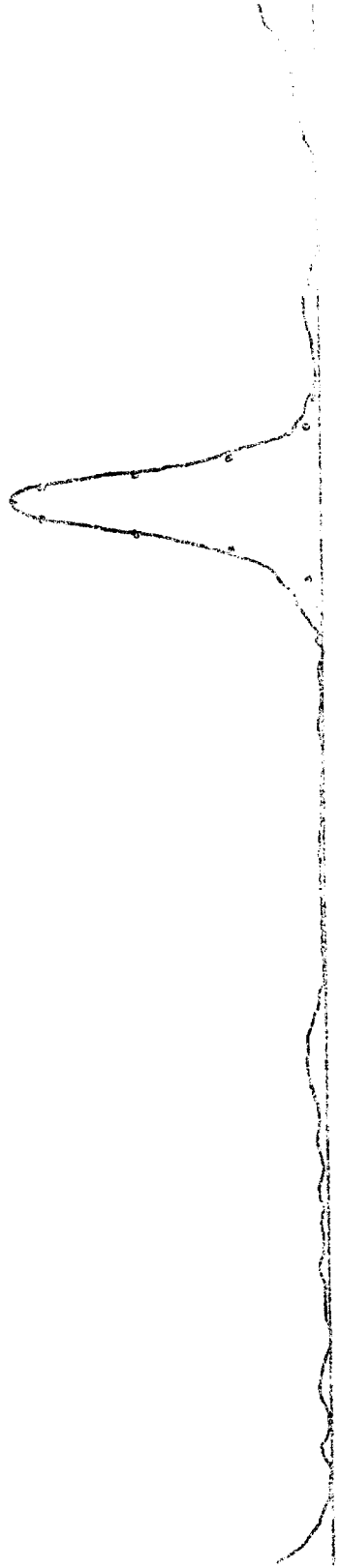
The following figures, prepared by B. J. O'Mara, show the fits to the profiles of lines of sodium and calcium. The logarithm of the abundance on the scale $\log N_H = 12.00$ is given for each line. The scatter is produced at least partly by uncertainties in the f-values. The broadening of the sodium lines arises almost entirely from electron collisions. Collisions also produce an asymmetry in the line which, for some transitions, is quite large. Note in particular the 4668.57 line of multiplet no. 12. In a number of examples, electron broadening does not suffice to account for the very extended line wings, e.g. λ6154.24 of multiplet no. 5. To account for the wings of such lines, it is probably necessary to take into account the quasi-static ion broadening. For a number of lines, the continuum is evidently depressed by numerous weak, small lines which may overlap one another.

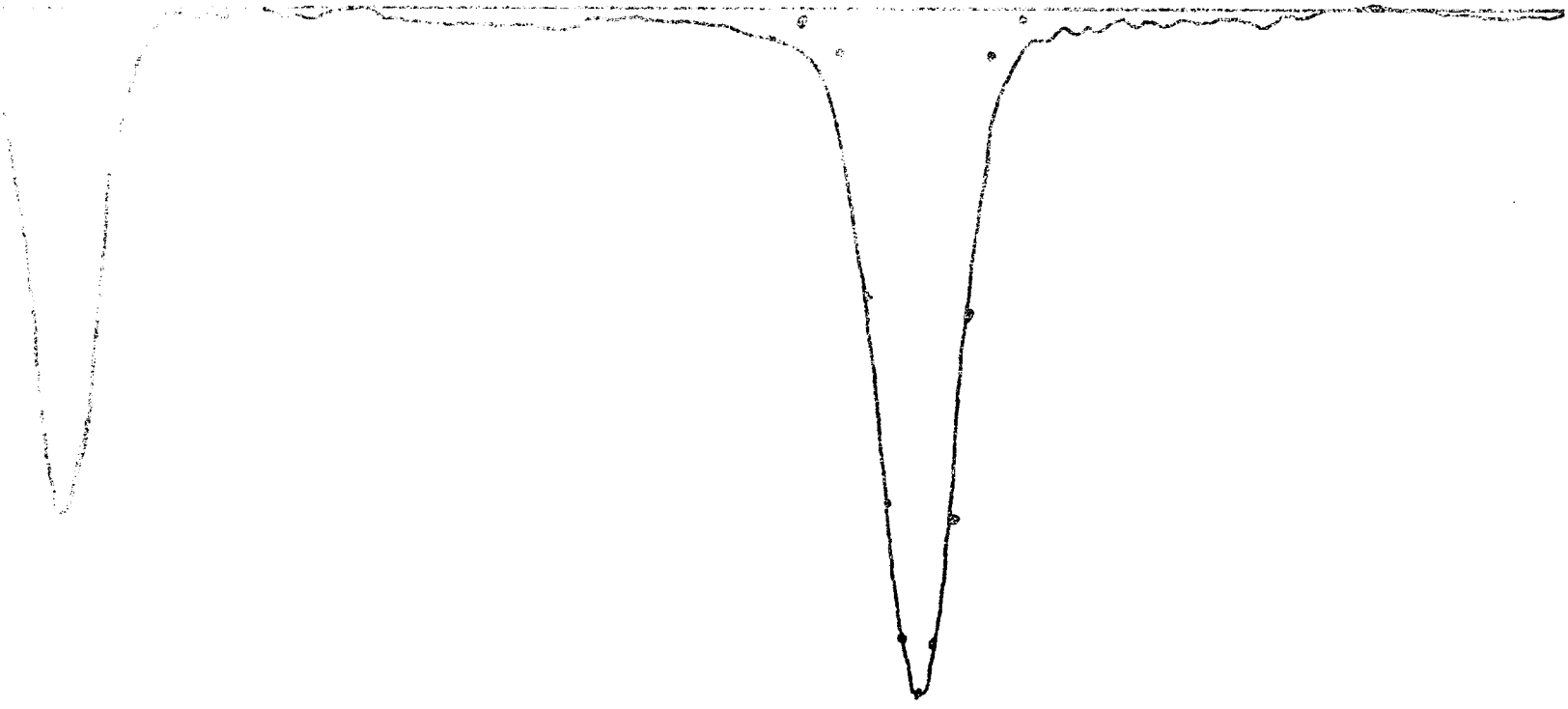
Apparently the broadening of the calcium lines is produced by van der Waals interactions, but the widths predicted by the Lindholm Foley theory are usually too small.


Na.6154.24(5)
ABUND. = 6.33

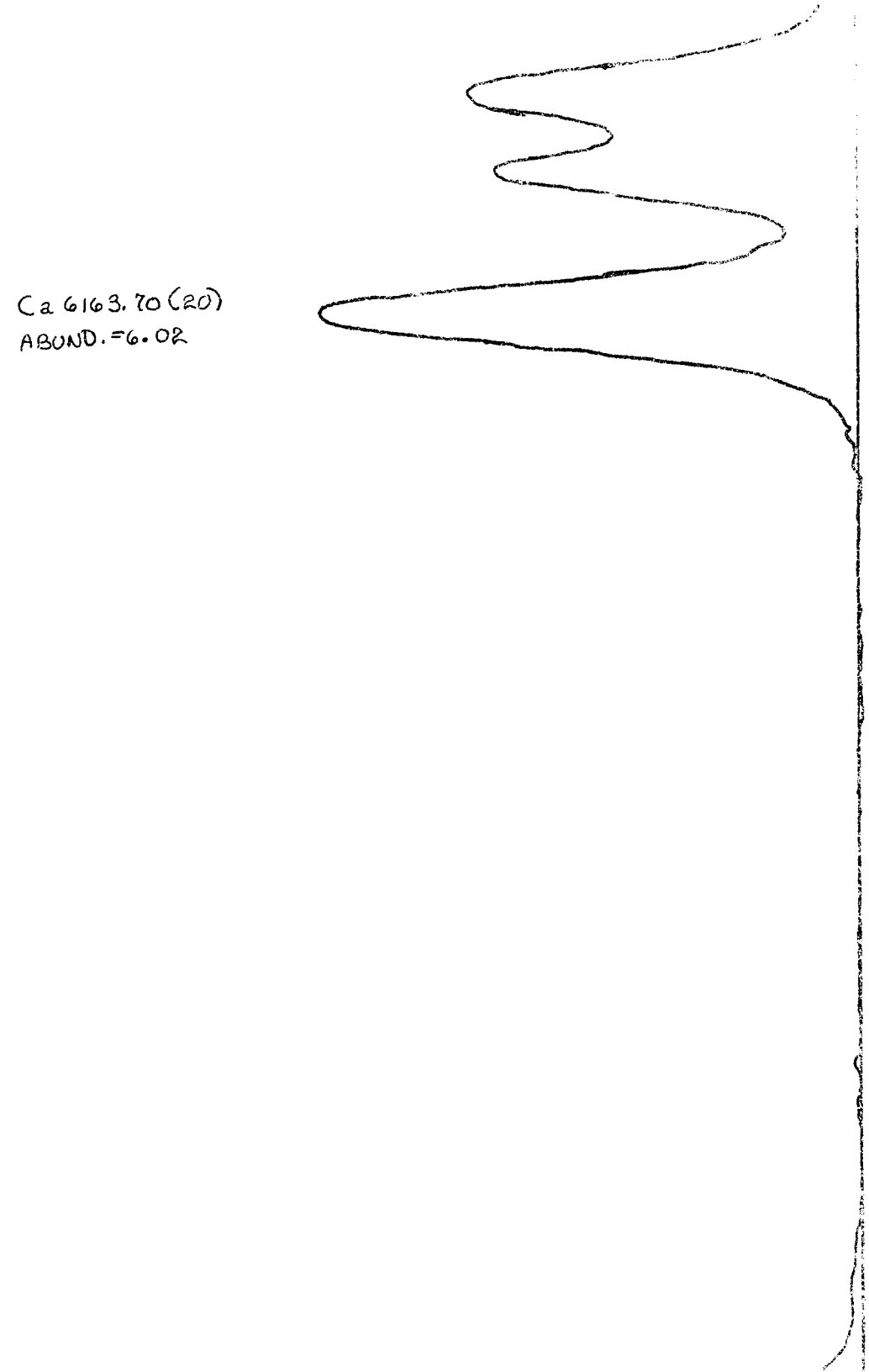

Na5682.22(6)
ABUND. =6.16


Na 4668.57(2)
ABUND. = 6.41


Ca6572.80(1)
ABUND. = 6.13



Ca 6166.45 (20)
ABUND. = 5.98

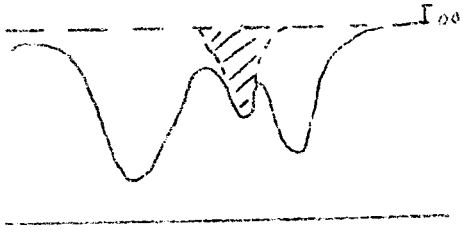

Ca 6163.70 (20)
ABUND. = 6.02

A determination of the abundances of rarer elements in the solar atmosphere involves a number of difficulties, viz:

(1) Since the abundances of the elements concerned are low, the spectral lines are weak eventhough they correspond to resonance lines with high transition probabilities.

(2) The lines often fall in heavily blended regions of the solar spectrum and the effects of neighboring lines therefore must be taken into account. There are two ways one may proceed.

(a) In the "curve of growth" method we assume that we know the rough shape of the line then extend the wings and measure the equivalent width. We take into account the effects of the overlapping of many weak lines in the neighborhood which tend to depress the continuum and use the combined effects of this "depression of the continuum" and limb darkening to evaluate an empirical background absorption coefficient, $K_\lambda(\text{emp})$ (see ref. 14).



Paul Mutschlecener in his thesis at Michigan (1962) employed this method to determine the abundances of lead, lithium, and beryllium, in the sun. We have employed it here as described below.

(b) In the "line profile method" one takes into account effects of neighboring lines according to a precise theory. In this way, it is possible to give a tailor-made treatment for each spectral line in the study and achieve a higher precision than is possible

by the older methods.

In the "curve of growth" approach one proceeds as follows: Rather than employing a weighting function procedure as was done by Unsöld and followed by many workers, one calculates an exact line profile. **The input data are:**

(1) The adopted model solar atmosphere

(2) Line data

(a) Identification (from which the program obtains such additional parameters as atomic mass, ionization potential, and partition function)

(b) Excitation potential of the lower level

(c) Wavelength

(3) Broadening function subroutine (Doppler broadening plus damping)

Our problem is to solve an equation of the form

$$W_\lambda = \int \int_{\tau=0}^{\infty} S_\lambda \, e^{-\tau_\lambda/\mu} \frac{d\tau}{\mu} \, d\lambda \qquad \tau_\lambda = \tau_\lambda^{\text{contin}} + t_\lambda$$

τ_λ^c being a function of the atmospheric model and t_λ a function of the model, element and the quantity $gf\lambda(n_{element}/n_H)$

In the continuum $t = 0$. Here S_λ is the source function. (see e.g. Greenstein "Stellar Atmospheres" Chap. 4).

Thus by integrating the residual intensity, ie. the profile of the line, we obtain the equivalent width, W_λ. If we plot $\lg W_\lambda/\lambda$ vs. $\log gf\lambda\ (n/n_H)$ we obtain the curve of growth. A plot of the observed $\log W_\lambda/\lambda$ against $\log gf\lambda$ then enables one to get the abundance of the element by a simple shift of abscissa, but we must know the $gf\lambda$ value for the line. All of this is the time-honored standard procedure.

It turns out that the curve thus obtained is a strong function of the atmospheric model and theline parameters. John Ross has employed what appears to be a more satisfactory approach.

Let us define $\log W^*_\lambda/\lambda = \log N/N_H + \log gf\lambda + \log C$

where log C involves the model atmosphere and the stratification effects. If we now plot $\log W^*_\lambda/\lambda$ against $\log W_\lambda/\lambda$ we obtain a "curve of growth" but the abscissa is shifted by an amount $\log gf\lambda C$. This curve is just as "exact" as the conventional curve, but the influence of the atmospheric model and line parameter dependences virtually vanishes.

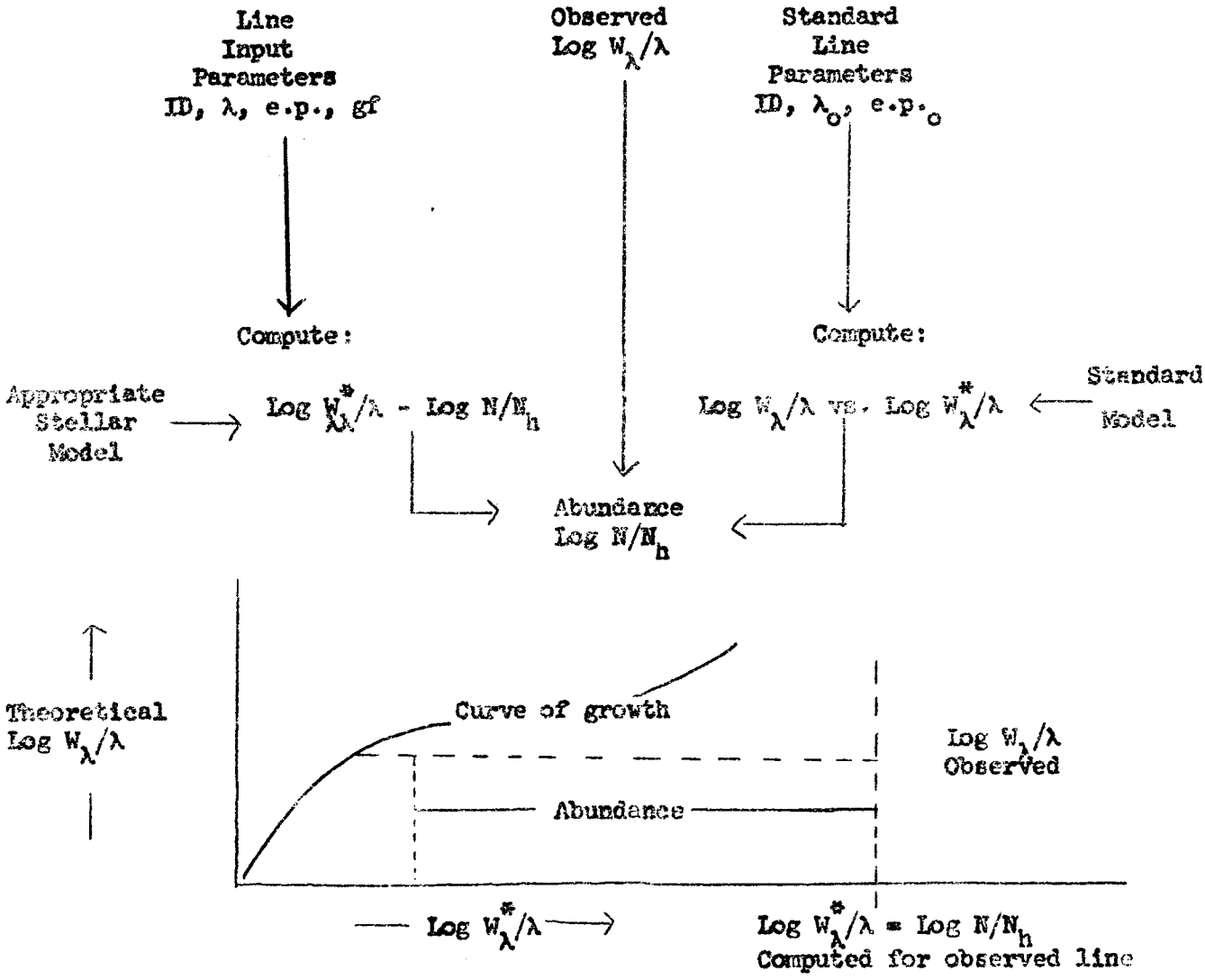
Calculation of the theoretical $\log W_\lambda/\lambda$ is quite involved and requires several seconds of time on the IBM 7094; the computation of $\log W^*_\lambda/\lambda$ is much easier.

Since the thus modified "curve of growth" which is actually a "saturation effect" curve is fairly independent of the model chosen and line parameters, one can compute a "standard" curve for some selected model and then use this curve for most of the lines of an element. In practice the error is less than a percent for weak to moderatley strong lines. The effect of the model still enters of course in the computation of $\log \frac{W}{\lambda} - \log \frac{N}{NH}$ for the individual lines.

The routine is indicated schematically in the following flow chart. First one chooses a set of "standard" line parameters appropriate to a standard model and computes $\log W^*_\lambda/\lambda$ and $\log W_\lambda/\lambda$, thus deriving a curve of growth.

Next, one selects input line parameters for the lines at hand and computes $\log W^*_\lambda/\lambda - \log N/N_H$ for appropriate model. Then from the observed $\log W_\lambda/\lambda$ and the theoretical curve the abundance is gotten.

The procedure can be applied to any star for which suitable model atmospheres exist.



The line profile or solar spectrum synthesis method

One great advantage in solar work is that one can observe the actual line profiles at various points on the solar disk and measure the emergent intensity $I_\lambda(0,\mu)$. Full utilization of the available data permits a much better determination of the quantity log gfλ (n/n_H) than does the curve of growth method.

It is possible not only to determine the abundance from an isolated line but also to handle the problem of blends. Consider a blended line, or more generally a region of the spectrum crowded by several recognizable discrete lines. The total absorptivity at some point in this interval will be

$$\kappa_{total} = \kappa_\lambda + \kappa_\lambda(emp) + \sum_i \left\{ \frac{\ell_\lambda}{gf\lambda\, N/N_H} \right\}_i \times gf\lambda \frac{N}{N_H}$$

Here κ_λ = continuous opacity arising from conventional contributors, atomic hydrogen, the negative hydrogen ion, and the more abundant metals.

$\kappa_\lambda(emp)$ = an empirical opacity arising from overlap of unrecognised lines and unidentified contributors of continuous absorption. It is evaluated by requiring the observed intensity at the center of the disk in the local continuum and the observed limb darkening to agree with theory. (see ref. 14)

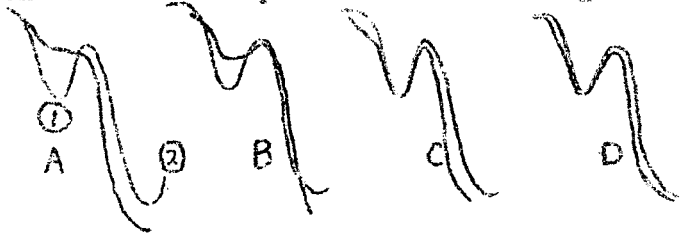
$\ell_{\lambda i}$ = absorption coefficient at frequency for the i-th line that contributes in the neighborhood.

$(gf\lambda N/N_H)_i$ = refers to data for this i-th line, including the abundance N/N_H of the element in question.

In principle we alter the $\kappa_\lambda(emp)$ and $(fN/N_H)_i$ until the computed (synthesized) region reproduces the observed region.

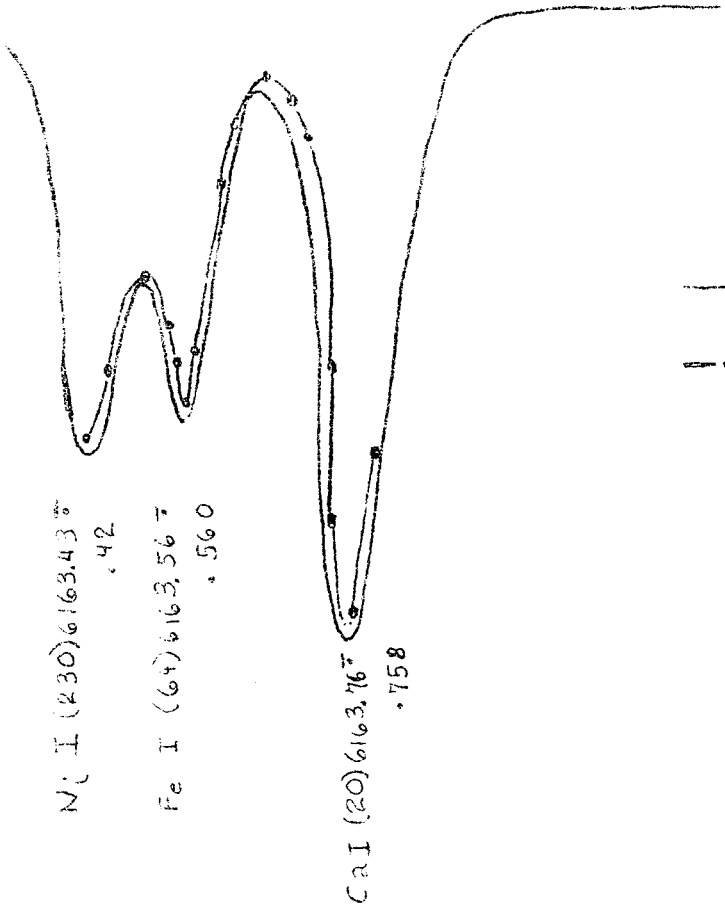
In an ideal situation, the abundances of the elements responsible for

the blending and the f-values would be known: in any event we can get a good estimate of starting values of the product fN/N_H from the curve of growth. Then we alter the product until the region has been synthesized.



A schematic example is shown herewith. "A" represents the initial guess, "B" and "C" are the results of increasing $gf\lambda\ N/N_H$ of line (1), then "D" is the final result after decreasing this quantity for line (2).

The sensitivity of the method is illustrated by a trial run in synthesis of a region near $\lambda 6163\text{Å}$. The effect of doubling the value of the adopted iron abundance (or more accurately the product $gf\lambda\ N_{Fe}/N_H$) is clearly shown.



Sample Synthesis of Region Near $\lambda 6163\text{Å}$.

——— Solid Curve is Observed Spectrum

—·—·— Is Synthesized Region with Previously Determined Values of $(gf\lambda\ N/N_H)$

Is Synthesized Region but with $(gf\lambda N_{Fe}/N_H)$ = Twice the Previously Determined Value.

Next, we show an attempt to synthesize the region of the λ3382.900 AgI line by the line profile method. The position of the background continuum $I_\lambda(0,0)$ is indicated at the top of the figure. It is calibrated in terms of absolute intensity from the data of Houtgast. The solid curve gives the observed intensity $I_\lambda(0,0)$ and the red curve the synthesized portions.

For this calculation, Ross adopted the Müller Mutschlecner model with a turbulent velocity of 1.8 km/sec, opacity arising from atomic hydrogen, the negative hydrogen ion and abundant elements Silicon and Magnesium. The damping constant for these lines was treated approximately by replacing the usual

$$a = \frac{\Gamma}{4\pi\Delta\nu_D} \qquad \text{by} \qquad a = \frac{10\Gamma_c\,\theta^{0.7}P_g/Q}{4\pi\Delta\nu_D}$$

where $$Q = \theta_0^{0.7}P_{g_0}$$

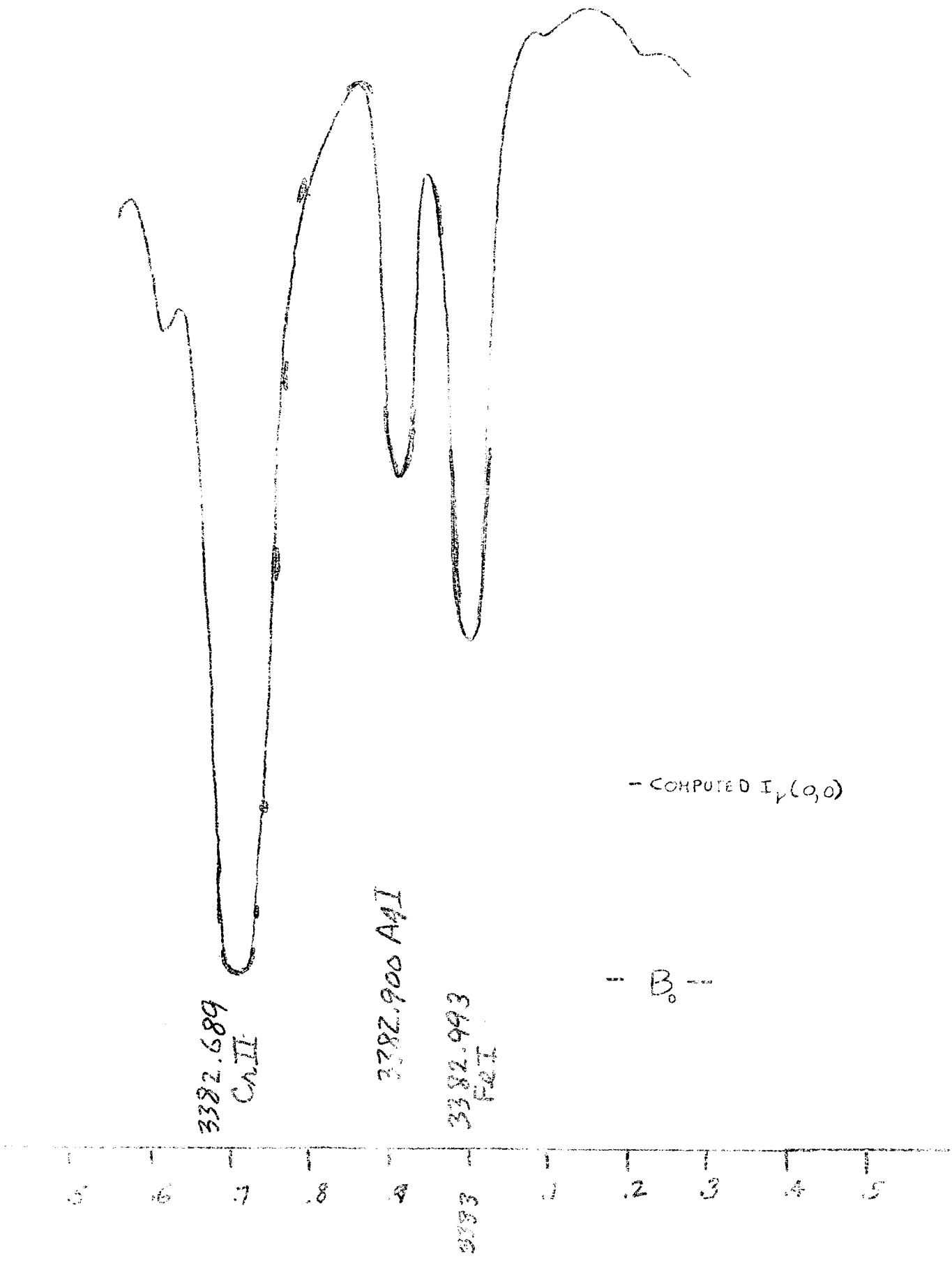
Then Γ is about 10 times larger then the classical value in the outermost atmospheric stratum. This result is somewhat better than setting a = constant and much better simply taking Γ to have a fixed value of $10\,\Gamma_c$. B_0 denotes the intensity corresponding to the boundary temperature.

The following data were required to represent the lines

wavelength of solar line	ion	$\log (gf\lambda\, N/N_H)_k$
3382.689	CrII	-11.05
3382.900	AgI	-16.15
3382.993	FeI	-10.35

In this instance three lines were required in the wavelength grid.

Each step in the synthesis required approximately one second of computing time.


3382.689
CrII
3382.900 AgI
3382.993
Fe I
- COMPUTED $I_\nu(o,o)$
- B_o -
.6
.7
.8
.9
.2
.3
.4
.5
3383

A comparison of the results is given in the following table

Investigation	log gfλ $\frac{N}{N_H}$	log gfλ (AgI λ3382.90) Allen -4.22	BD -4.72	f-sum rule -4.69	NBS -4.75	LLK -4.84
GMA (ref. 12)	-4.16	+0.06	+0.56	+0.43	+0.59	+0.68
"curve of growth"	-4.22	+0.00	+0.50	+0.47	+0.53	+0.62
synthesis	-4.15	+0.07	+0.57	+0.54	+0.60	+0.69

The references for gfλ are as follows:

Allen, C. W. 1957, M.N.R.A.S. 117, 622 (GMA ref. no. 4)

Bates, D. R. and Damgaard, A. 1949, Phil. Trans. Royal Soc. London, A, 242, 101 f-sum rule - see GMA, p. 8

NBS = Corliss, C. and Bozman, W. R., National Bureau of Standards Monograph 53, 1962

LLK = Lawrence, G. M., Link, J. B. and King, R. B., 1965, Ap.J. 141, 293

In this instance the difference between the results obtained by the three methods is very small, largely because the effects of blending could be allowed for largely by eye. The hypothetical unperturbed profile could be estimated rather easily. The comparison shows another feature to which we shall return later, namely the effects of uncertainties in the f-values mask the errors which may arise from the uncertainties in the model or theoretical treatment.

Comments on analyses by curve of growth method

Introduction:

This metal has a fair number of rather weak, often badly blended lines. The data were carefully re-examined by Courtney Seligman; in many cases the equivalent widths differed from those obtained by GMA.

Summary of data for the curve of growth

λ	log W_λ/λ	log gfλ	abcissa
3436.737	-5.78 ± 0.03	-4.35	5.27
3498.946	-5.35 ± .02	-4.41	5.39
3708.903	-5.58 ± .06	-4.48	5.01
4057.796	-6.09 ± .20	-4.52	4.19
4199.902	-5.00 ± .04	-3.96	5.02
4554.536	-6.06 ± .30	-4.19	4.79
4669.977	-6.56 ± .42	-6.02	2.83
4709.507	-6.37 ± .30	-4.53	4.11
4869.153	-6.26 ± .20	-5.17	3.68
5636.241	-6.35 ± .36	-5.46	3.04

Remarks on some of the lines

λ3436.737 There is a difference between the equivalent width derived from these data and those given by GMA.

λ3498.946 The revised value for the equivalent width is smaller than the GMA value.

λ3593.017 This line is too badly blended to be of any use in the analysis. Likewise, λ3794 is also not suitable and has been rejected.

λ3708.903 Again a revision of the profile measurements gives an equivalent width smaller than the GMA value.

λ3784.84 Could not be measured

λ4057.796 Seems to be satisfactory

λ4554.536 Seems to be OK, although there was a large scatter in the measured equivalent widths due to the complex character of the background.

λ4669.977 Is a difficult line, being both weak and blended, although the blending appears to be amenable to corrections.

λ5040.7 Is too badly blended to be of use

λ5171.023 Is strongly affected by blending of neighboring lines; it appears that the best procedure is to discard this line. If we had no other data we could use this line to obtain a minimum W_λ.

The final curve of growth shows a considerable scatter and without a great deal of further analysis improved values cannot be obtained. The NPS f-values have been used throughout.

It is estimated that the abundance lies in the range (log N_H = 12.00)

$$1.36 < \log N < 1.83$$

and we adopted log N = 1.59 as the most probable value. A spectrum synthesis would not be justified until improved f-values are available.

The abundance of Indium

Indium is of considerable geochemical interest since it appears to be depleted in meteorites. Should this element be found on the moon, it would indicate an early history of lunar material considerably different from that of chondrites.

One good line of this element falls in a relatively uncrowded region of the spectrum at λ4511.34 (see accompanying trace). The equivalent width as measured by Geraldine Duffner on the newer Michigan material is 3.5mA, which is somewhat greater than the GMA estimate. She suggests a lower limit of 2.9mA. The higher abundance of indium can be attributed almost entirely to the difference in equivalent widths which arises from differing estimates of the position of the continuum. The problem needs to be re-examined by the line profile method.

The best estimate of the solar abundance of indium would appear to be Log N (In) = 1.4 (log N_H = 12.00) but uncertainties in both the f-value and in the equivalent width enter the picture.

Indium Abundance

λ 4511

	log $\frac{}{\lambda}$	log $gf\lambda\frac{N}{N_H}$	log N for log (gfλ) = -4.53 CB	log N for log (gfλ) = -4.41 OPS
GMA	-6.40	-3.25	1.28	1.16
Duffner(a)	-6.12	-2.96	1.57	1.45
(b)	-6.19	-3.03	1.50	1.38

CB = Corliss Bozman NGS 53

OPS = (GMA ref no. 79.04) Ostrovosky, Penkin and Shabanova, Izv. Akad. Nauk USSR, Ser Phys, 22, 6, 725.

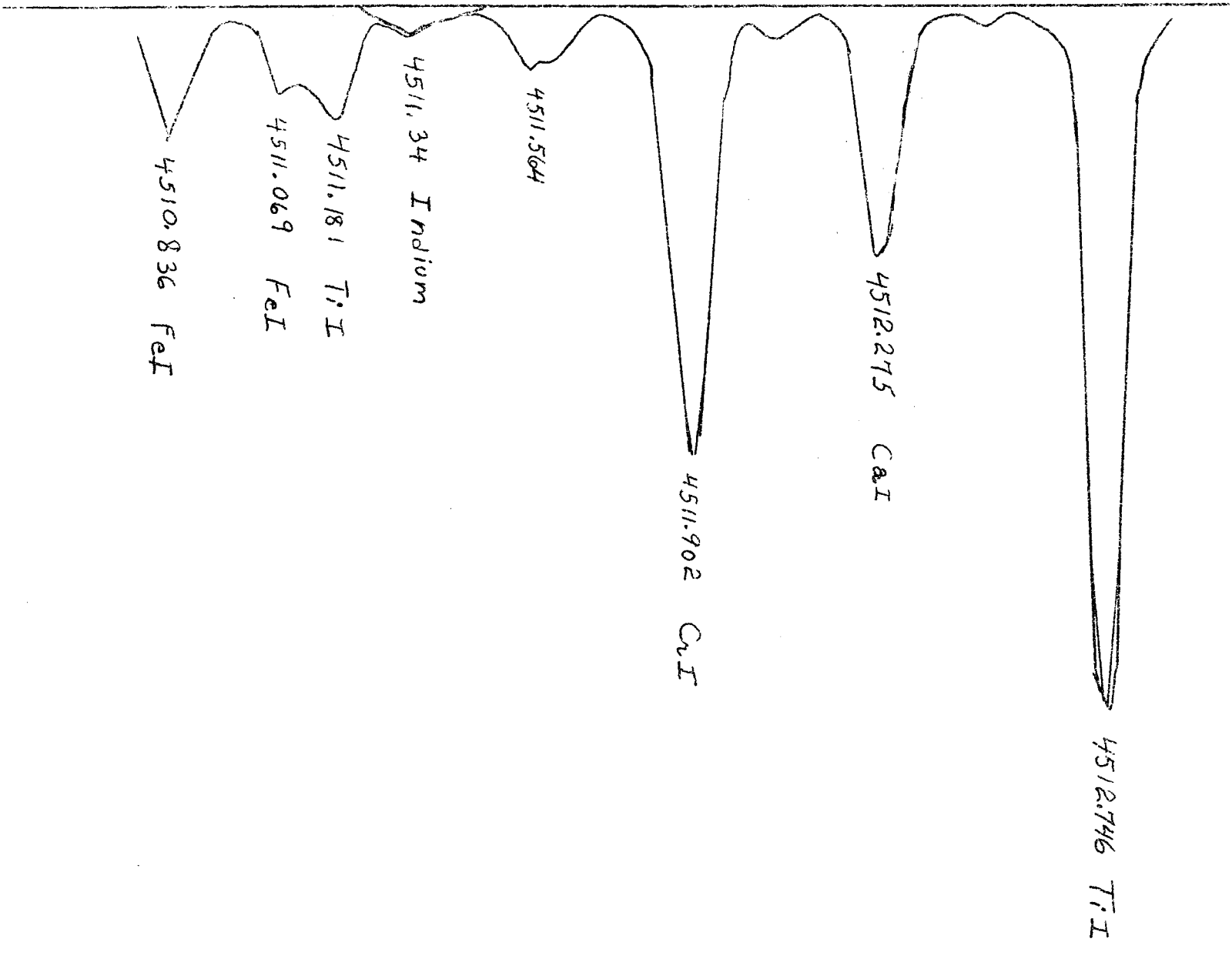
(a) most likely value

(b) lower limit

The solar abundance of gold

The available gold line lies in the far "accessible" ultraviolet at λ3122.784. The big problem here is locating the regional continuum, calibrating the same in terms of energy units, and allowing for effects of blends. Only our "curve of growth" method has been employed: spectrum synthesis has not been attempted yet in this region. Miss Duffner obtained an equivalent width of 3.1 mA from which is obtained a gold abundance log N(Au) = 0.32

Indium in the Solar Spectrum



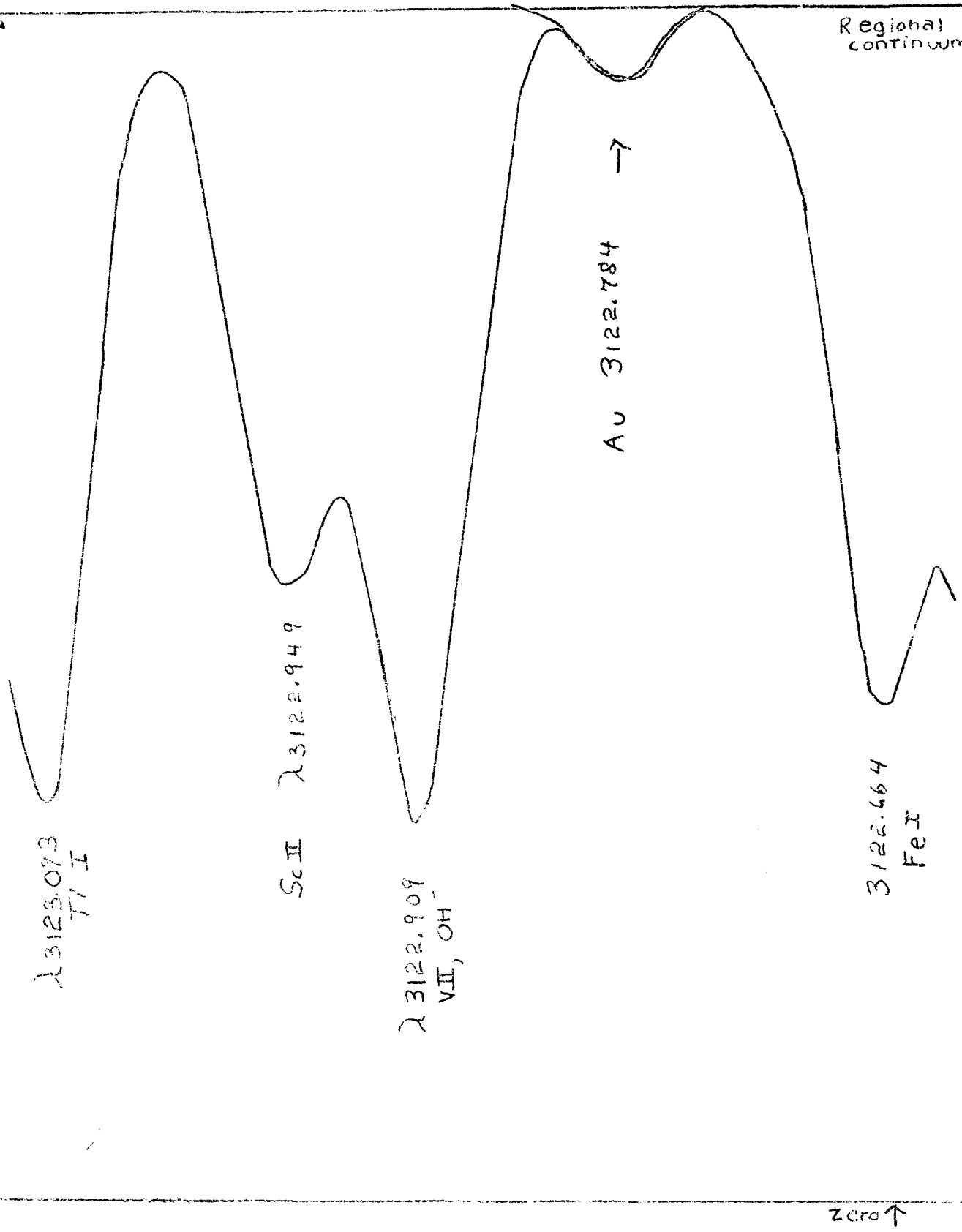
The problem of the atomic transition probabilities

Whether one uses the solar spectrum synthesis or the "curve of growth" method the result of the analysis is an evaluation of the product, fN_{el}/N_H where N_{el}/N_H is the quantity sought, and f is the oscillator strength for the transition in question. The final value for the abundance can be no better than the accuracy of the f-value.

Transition probabilities can be evaluated either by experimental methods or theoretical procedures (7). In spite of many attempts, large uncertainties still persist. In this investigation we have relied on a combination of experimental and theoretical results. Whenever they were available we have used f-values measured by R.B. King and his associates at the California Institute of Technology. We have also made extensive use of the new f-values published by Corliss and Bozman at the National Bureau of Standards, but it now appears that their results will have to be revised for a number of elements.

One possible procedure that we would like to examine is to employ stellar spectroscopic data to improve available transition probabilities. That is, from accurate measurements of line intensities in the spectra of stars (wherein the lines in question are unblended), one can obtain seemingly reliable relative transition probabilities which can be put on an absolute scale as soon as the absolute f-values of a few of the lines have been established. We propose to do this particularly for the lines of ionized metals of the iron group, whose transition probabilities are extremely difficult to measure in the laboratory. If one can measure the abundance of an element from lines in two stages of ionization, e.g. the chromium abundance from lines of CrI and CrII, he can assess to what

GOID IN THE SOLAR SPECTRUM



extent such factors as deviations from local thermodynamic equilibrium play a role.

For some elements, it is possible to calculate apparently reliable f-values. Such calculations are possible for the lighter elements, e.g. aluminum and magnesium whose lines are prominent in the solar spectrum. The abundances of aluminum and magnesium are of considerable interest. Dr. Robert Chapman has undertaken the difficult task of calculating accurate transition probabilities, using accurate, numerically evaluated wave functions.(15)

The procedures employed are adapted from those developed by Stanley Cayzak and his associates. The current goal in this program of computing Hartree-Fock self-consistent field wave functions is to produce results for the configurations:

$1s^2 2s^2 2p^6 3s^2 3p$, 3d, 4s, 4p, 4d, 4f, 5s, 5d, 6s, 6p, 7s

in the first three ions of the isoelectronic sequence Al, Si^+, P^{++}. Once these simple configurations are completed, we will look at the more complex cases of the configurations in which one of the two 3s electrons is also in an excited state, in addition to the outermost electron.

At present, we have successfully obtained 3p wave functions for the three ions and 4s wave functions for Si^+ and P^{++}. The 4s configuration for neutral aluminum has presented us with difficulties, which only now are being cleared up. Severe convergence difficulties appeared, but with the aid of assistance from S. J. Cayzak, we were able to obtain appropriate self-consistent wave functions and can now attempt to complete the present phase of the project.

Once the wave functions are obtained, we will compute transition probabilities for the spectrum lines of astrophysical interest. In obtaining the transition probabilities, we must include some means of evaluating the effects of configuration interaction. Appropriate means of including this effect are being studied.

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