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THE CALCULATION OF THEORETICAL CHROMOSPHERIC MODELS AND PREDICTED OSO I SPECTRA

NASA Grant NSG-7054

Progress Report No. 1

For the period 1 July 1974 to 31 December 1975

Principal Investigator
Eugene H. Avrett

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March 1976

Prepared for
National Aeronautics and Space Administration
Washington, D.C. 20546

Smithsonian Institution
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The Smithsonian Astrophysical Observatory
and the Harvard College Observatory
are members of the
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The NASA Technical Officer for this grant is Dr. Adrienne F. Timothy, Code SG, Headquarters National Aeronautics and Space Administration, Washington, D.C. 20546

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ABSTRACT

We report our progress in computing theoretical solar chromospheric and photospheric models for use in analyzing OSO 8 spectra. We have updated the Vernazza, Avrett, and Loeser (1976) solar model and produced self-consistent non-LTE number densities for H I, He I, He II, C I, Mg I, Al I, Si I, and H^-. These number densities have been used in the calculation of a theoretical solar spectrum from 90 to 250 nm, including approximately 7000 lines in non-LTE. More than 60,000 lines of other elements were treated with approximate source functions.

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1. INTRODUCTION

The OSO 8 experiment has observed radiation from different regions on the solar disk and, through spectrum scans, has probed a range of depths in the atmosphere from the corona to the upper photosphere. These observations, together with earlier Skylab and rocket observations, should lead to a new and greatly improved understanding of the structure and behavior of the solar atmosphere and of the heating of the corona, as well as to significant advances in our theoretical understanding of high-temperature plasmas.

The variation with depth of temperature, density, and other atmospheric parameters at a given point on the disk can be determined from the emergent spectrum. However, the computations necessary to derive these parameters require a major effort. We have developed a two-stage procedure for computing theoretical solar chromospheric and photospheric spectra. In the first, we construct a solar model based on the non-LTE computer program PANDORA (see Avrett and Loeser, 1969; Avrett, 1971; Vernazza, Avrett, and Loeser, 1973).

In the second stage of the spectrum calculation, we make use of a spectrum-synthesis program written by Kurucz (1974) and based upon his model atmosphere program ATLAS (1970), which includes data for 300,000 lines computed by Kurucz and Peytremann (1975). The statistical-equilibrium number densities from the model calculation are used to determine the non-LTE line source functions of the abundant elements, while the less abundant ones are treated with approximate source functions.

In the next section we describe our current solar model; and in section 3 we outline various developments in the spectrum synthesis program, especially the treatment of lines merging into continua and non-LTE modifications to the basic programs. In sections 4 and 5 our spectrum calculations are described. Finally, we discuss further work to remedy shortcomings in the most recent calculations.

2. SOLAR MODEL

We construct a solar model by choosing a temperature-height distribution such that the computed emergent intensity is in best agreement with observed line and continuum spectra in the ultraviolet, visible, and infrared spectral regions. PANDORA is used to solve the radiative-transfer and statistical-equilibrium equations for hydrogen, helium, carbon, silicon, and other important constituents. The model calculation is iterative in that only one atom can be computed at a time, while others are held fixed. Thus a self-consistent solution is found by cycling through the atoms several times, updating the number densities with each calculation.

Vernazza, Avrett, and Loeser (1976) have completed a detailed study of the solar continuous spectrum redward of 125 nm. They have constructed a temperature-density model, which is a representation of the quiet solar atmosphere in the height range between the photosphere and the chromosphere-corona transition region. We have revised and improved that model to obtain the temperature-height relation shown in Figure 1. The model is self-consistent in H I, He I, He II, C I, Mg I, Al I, Si I, and H^-.

We expect to further revise this model by studying the differences between our calculated spectrum and the rocket and OSO observations all through the ultraviolet and the Skylab spectra below 140 nm.

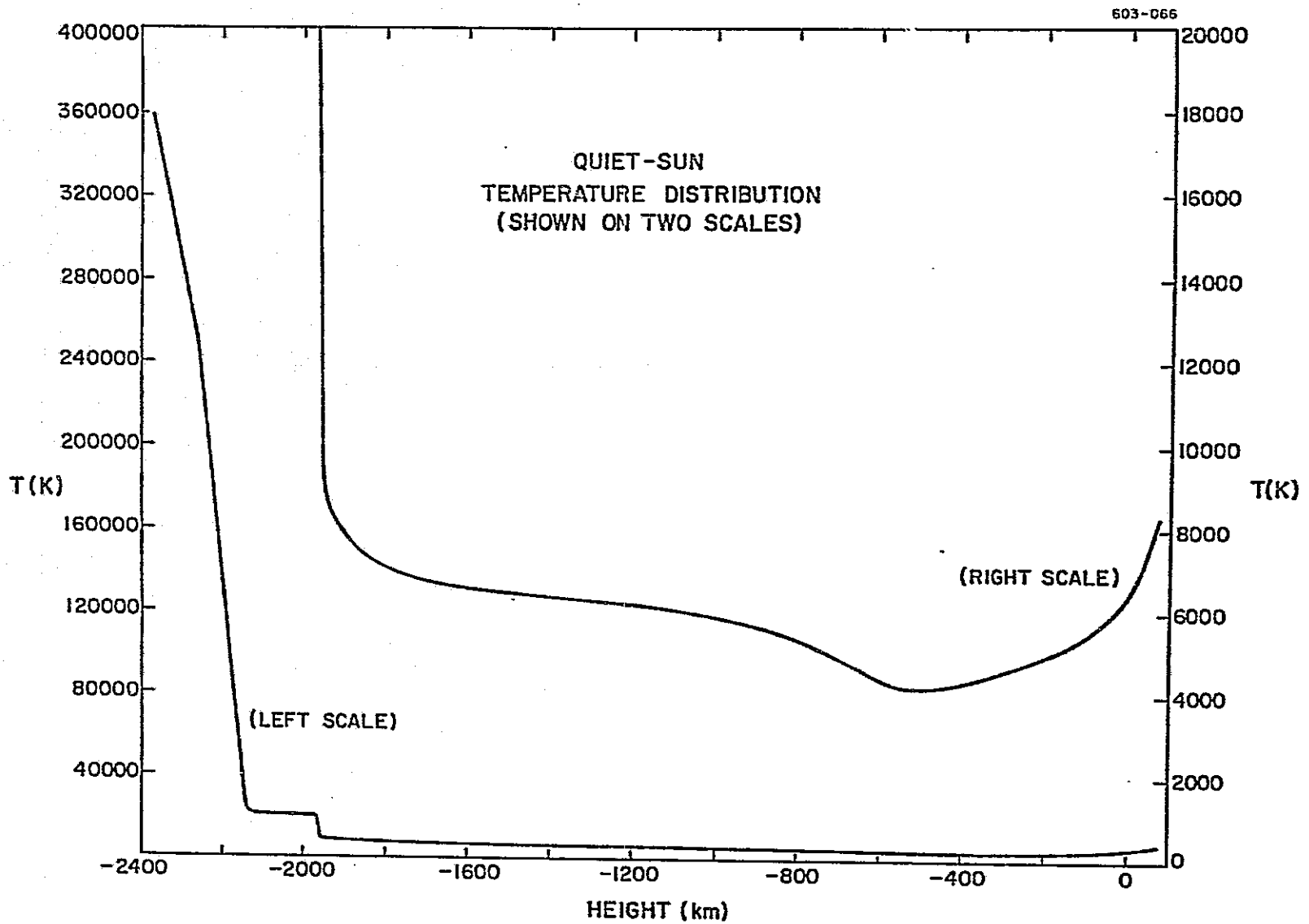

Figure 1. The temperature-height relation for our revised solar model.

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3. SPECTRUM SYNTHESIS PROGRAM

We have continually improved our spectrum synthesis programs during the course of this research. The basic spectrum synthesis program works as follows. For a given model atmosphere tabulated at 40 depths, we compute number densities and partition functions for all atoms and ions. Then we read the magnetic tape that lists the gf values calculated by Kurucz and Peytremann (1975), and compute a line opacity spectrum at each depth. The expressions for radiative, Stark, and van der Waals broadening are

$$\Gamma_R = \Gamma_{classical} = 2.223E13/\lambda^2 \quad , \qquad \lambda \text{ wavelength in nm} \quad ;$$

$$\Gamma_S = 1.0E{-8}\, n_{eff}^{\ 5}\, N_e \quad ;$$

$$\Gamma_W = 4.5E{-9}\, \langle r^2 \rangle^{4/10}\, [N_H + 0.42\, N_{He} + 0.85\, N_{H_2}]\, (T/10000)^{3/10} \quad ;$$

where

$$\langle r^2 \rangle = 2.5\, n_{eff}^{\ 2}/Z_{eff}^{\ 2} \quad ,$$

$$n_{eff}^{\ 2} = R\, Z_{eff}^{\ 2}/E_{up} \quad ,$$

Z_{eff} is the charge plus 1, E_{up} is the upper level energy, and R is the Rydberg energy. Next the continuum opacities, source functions, and intensities are evaluated at several points in the wavelength interval. The continuum quantities are interpolated to each point in the spectrum; the line opacity is added; the source function is approximated by

$$[(\kappa + \sigma) S_{cont} + \ell\, S_{line}]/(\kappa + \sigma + \ell) \quad ;$$

and the emergent spectrum is computed. Here κ and σ are the continuous absorption and scattering coefficients, ℓ is the line absorption coefficient, S_{cont} is the continuum source function including scattering, and S_{line} is the line source function, which is assumed to be the Planck function.

The following improvements have been made. We have computed mean square radii for the 4p orbitals of the iron group atoms and ions, and produced an interpolation formula

$$\langle r^2 \rangle = (45 - A + Z)/(Z + 1)$$

where A is the atomic number and Z is the charge. This expression is used for van der Waals broadening of all iron group atoms, assuming that the strong lines are all resonance lines with a 4p upper state.

There is now provision for additions, deletions, and corrections to the table of gf values and for use of individual "real" radiative, Stark, and van der Waals damping constants for each line.

To resolve the contribution of individual lines to blends, we now compute, in addition to the spectrum, the central intensity for each line in isolation.

We automatically produce spectrum plots with identifications.

The two most important advances as far as improving the appearance of the calculated spectrum have been treatment of lines merging into continua and the development of a procedure for computing thousands of lines in non-LTE.

One of the obvious faults in the preliminary calculations made one year ago was that strong discontinuities appeared at the C I, Si I, Al I, and Mg I edges, whereas the real spectrum makes smooth transitions from one continuum to another because in the real spectrum there are numerous lines that gradually merge into each continuum. In rewriting the opacity routines to include departures from LTE as discussed below, photoionization continua were put in for level-to-level transitions rather than

for term-to-term transitions as was the case previously. Thus, for example, for C I and Si I, ionization from the neutral ground term ^3P to the ionized ground term ^2P actually forms 6 continua, $^3P_0 \rightarrow {}^2P_{1/2}$, $^3P_0 \rightarrow {}^2P_{3/2}$, $^3P_1 \rightarrow {}^2P_{1/2}$, $^3P_1 \rightarrow {}^2P_{3/2}$, $^3P_2 \rightarrow {}^2P_{1/2}$, $^3P_2 \rightarrow {}^2P_{3/2}$. Each of these continua has a series of lines converging up to it. The lines merge into a quasi-continuum at an upper energy or upper quantum number determined by Stark broadening, because lines are no longer visible when the Stark width exceeds the line spacing. In practice, at each depth in the atmosphere, we compute the energy at which individual lines are no longer visible and extend each continuum redward at a constant level to this point. This technique smooths the transition from one continuum to another even if no lines are included explicitly.

For Al I and Mg I we were able to compute Rydberg series to high n (80), and to find or estimate the radiative, Stark, and van der Waals broadening for each line. For Si I and C I there is so much configuration interaction that extrapolated energy levels can be off by up to 2 cm^{-1} unless great effort is made to include the interaction effects, so we were not able to compute the series. For Si I, however, energy levels have been observed up to n = 56 although many of them were unclassified. We were able to pick out the interacting levels by estimating the mutual repulsion, so we could assign each level to an LS series. Then we estimated LS f values by extrapolating each series. These f values will be correct for many of the lines but wrong for the strongly interacting lines. However, the total f values spread over all transitions should be correct as configuration interation only redistributes the line strengths.

To demonstrate the improvement in the new calculations we show in Figure 2 sample old and new spectra calculated around the Si I edge at 198 nm. The old calculation predicted an abrupt discontinuity, and the new one, a gradual slope, in agreement with the observations.

To treat the non-LTE effects we have rewritten ATLAS (Kurucz, 1970) routines for partition functions and for continuous opacity from H I, He I, He II, C I, Mg I, Al I, and Si I to produce non-LTE populations, opacities, and source functions. We have added a new line opacity routine that produces non-LTE opacity and a source function for each C I, Mg I, Al I, and Si I line. The changes were accomplished by inserting departure coefficient b's as follows.

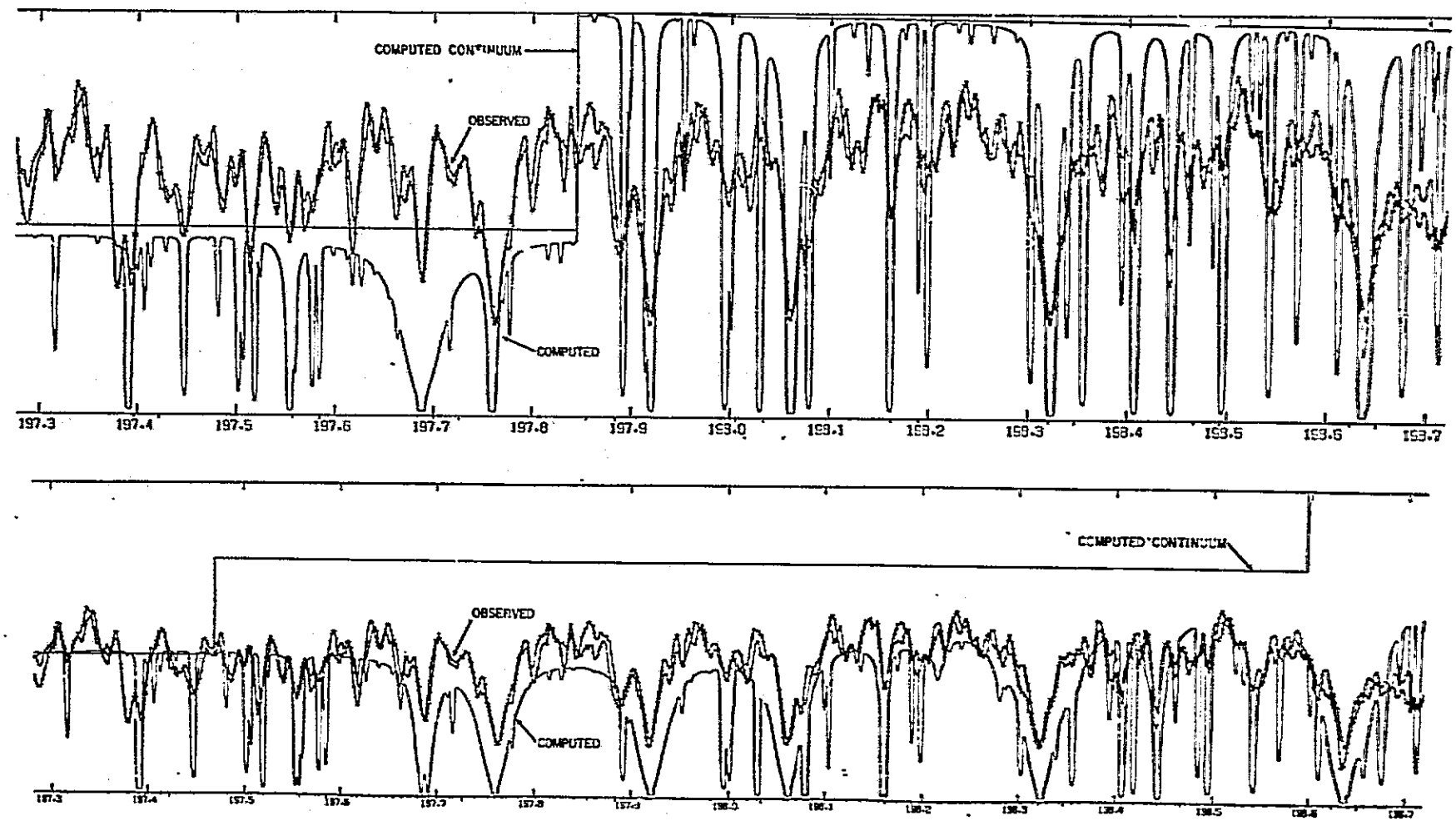

Figure 2. (a) A previous calculation showing the silicon discontinuity at 197.8 nm. Also shown are two Harvard rocket scans by Kohl, Parkinson, and Reeves that do not show an abrupt discontinuity. The vertical scale is linear but in arbitrary units. (b) Our most recent calculation showing the smooth transition across this region, in agreement with the observations, which results from treatment of lines merging into the continuum.

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Partition functions:

$$U = \sum g_i \, e^{-E_i/kT} \rightarrow \sum g_i \, b_i \, e^{-E_i/kT}$$

where g_i and E_i are the statistical weight and energy for each level:
Boltzman factors:

$$\frac{N_i}{N} = \frac{g_i}{U} e^{-E_i/kT} \rightarrow \frac{b_i g_i}{U} e^{-E_i/kT} \quad .$$

where N and N_i are the total and level number densities;
Stimulated emission:

$$1 - e^{-h\nu/kT} \rightarrow 1 - \frac{b_{up}}{b_{lo}} e^{-h\nu/kT}$$

where up and lo refer to the upper and lower levels. For ionization, up refers to the ground state of the ion.
Source functions:

$$S(lo \rightarrow up) = \frac{2h\nu^3}{c^2} \left[e^{h\nu/kT} - 1 \right]^{-1} \rightarrow \frac{2h\nu^3}{c^2} \left[\frac{b_{lo}}{b_{up}} e^{h\nu/kT} - 1 \right]^{-1} \quad .$$

In practice, b's are calculated only for the lowest 6 to 10 terms, so for higher levels b's are assumed to have the same value as the b for the lowest level of the ion.

4. COMPUTING TIME AT NCAR

This work on spectrum synthesis has been exceedingly difficult, requiring innovations and much more sophisticated programing than originally envisioned. Furthermore, calculation of the spectrum in non-LTE requires a great deal of computer time, even for debugging. Because of limited funds provided by the grant for computing, we have to use free computing where available. Fortunately we have been able to use the CDC 7600 at the National Center for Atmospheric Research through collaboration with Oran R. White of the High Altitude Observatory. A considerable inconvenience of working at NCAR is that to check the calculations we must bring magnetic tapes back to Cambridge to plot the spectra because NCAR does not have plotting facilities.

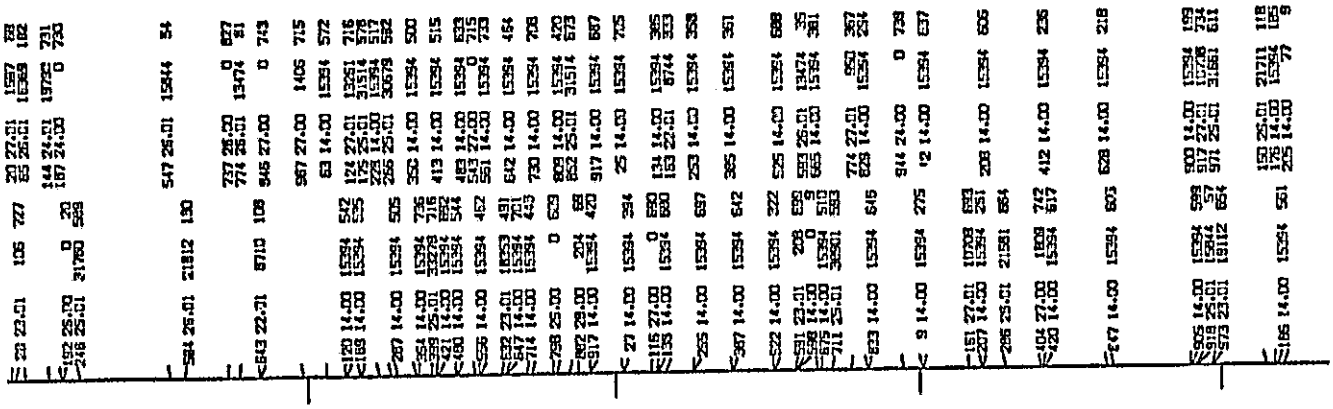
5. SPECTRUM CALCULATION

We used the model described in section 2 and the program described in section 3 to compute the theoretical solar spectrum from 90 to 250 nm including non-LTE effects for H I, He I, C I, Mg I, Al I, Si I, and H^-. We computed approximately 7000 lines in non-LTE. More than 60000 lines of other elements were treated with approximate source functions.

In Figure 3 we show an enlargement of Figure 2b with line identifications. Of the many lines included in the calculation, only those with residual intensities less than 0.99 are indicated. There are numerous non-LTE Si I lines in this region. The lines that show up prominently with triangular shapes in both the observed and calculated spectra are Si I resonance lines.

In Figure 4 we show a small region of chromospheric spectrum at 149.3 nm where the lines appear in emission.

Figure 3. The calculated spectrum compared to the Harvard rocket spectra of Kohl, Parkinson, and Reeves for the region 197.6 to 199.1 nm. The observed and computed spectra are not plotted on the same vertical scale; the two scales are linear but arbitrary. This figure shows approximately the same wavelength region as Figure 2b but enlarged to show detail and with line identifications added. The identifications at the top of the figure include: the last three digits of the wavelength, the element identification and charge (atomic number before decimal point, charge after; thus 14.00 = Si I and 28.01 = Ni II), then, the lower energy level in cm^{-1}, and finally the fraction of the full scale in per mil for the center of each line if it were in isolation. Thus strong lines have small central intensities and weak lines have values near the continuum, which is indicated. The numerous Si I lines are computed in non-LTE.



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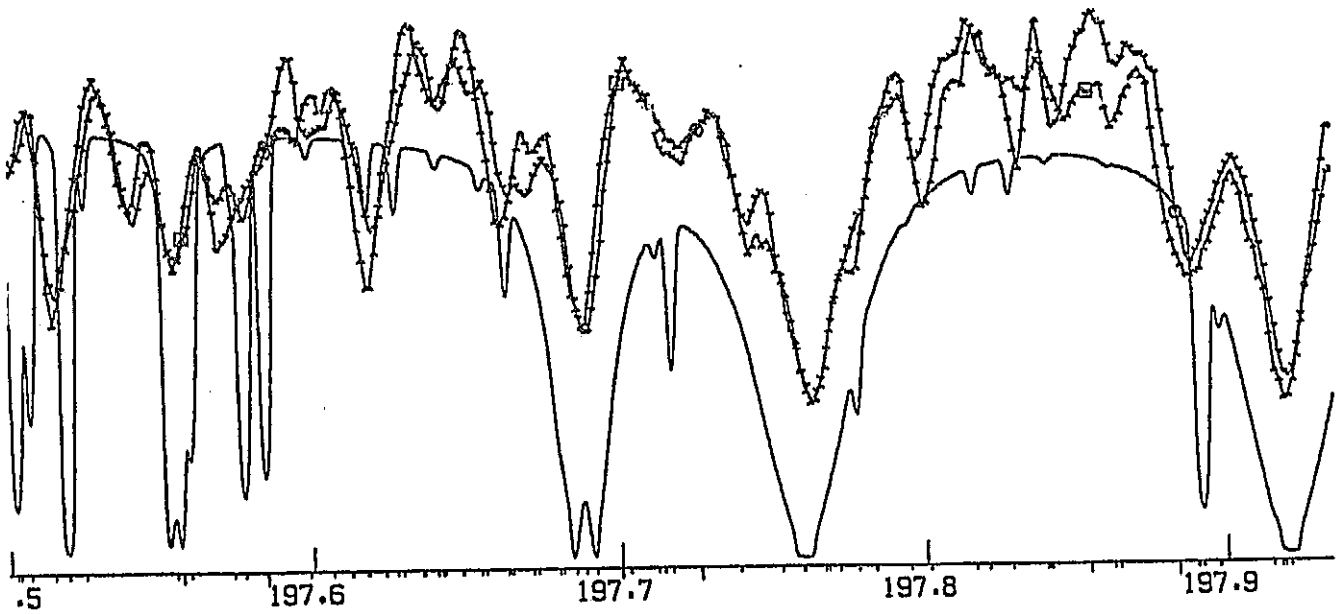

Figure 3.

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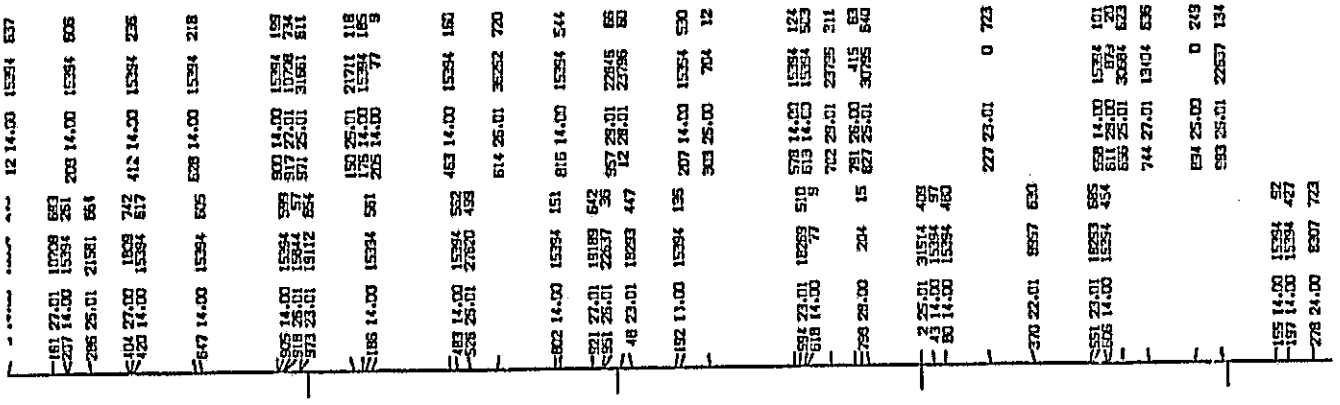
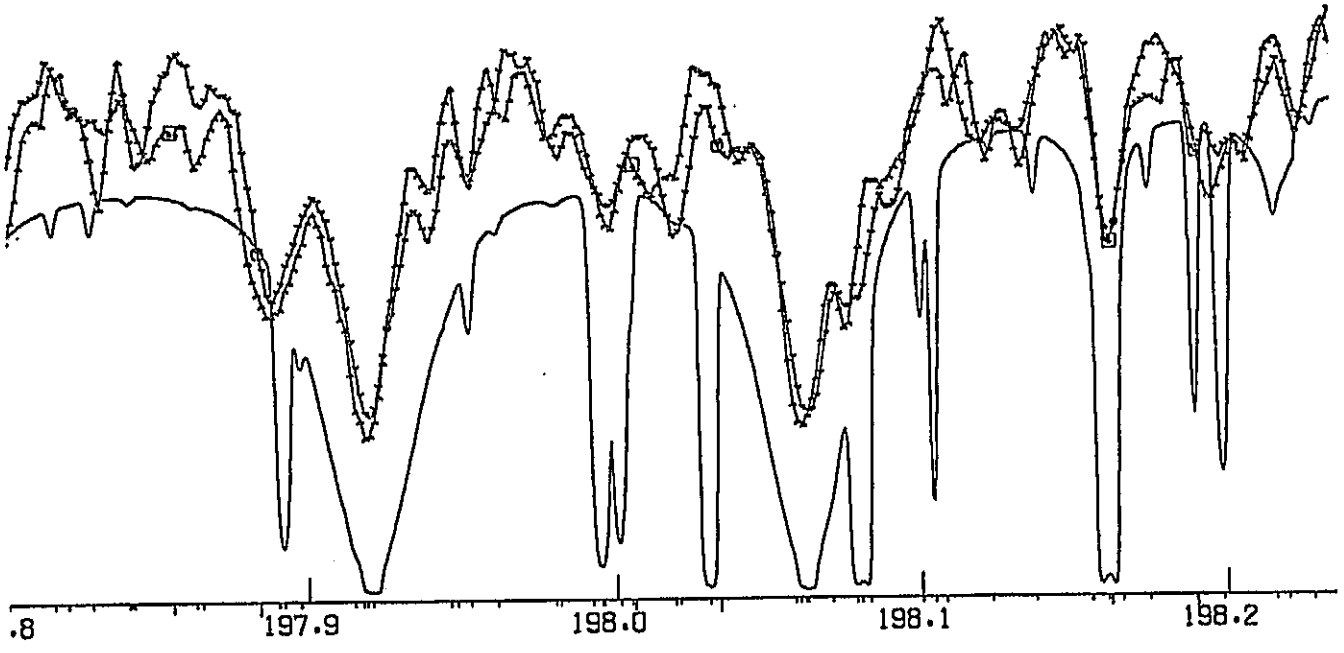


continuum



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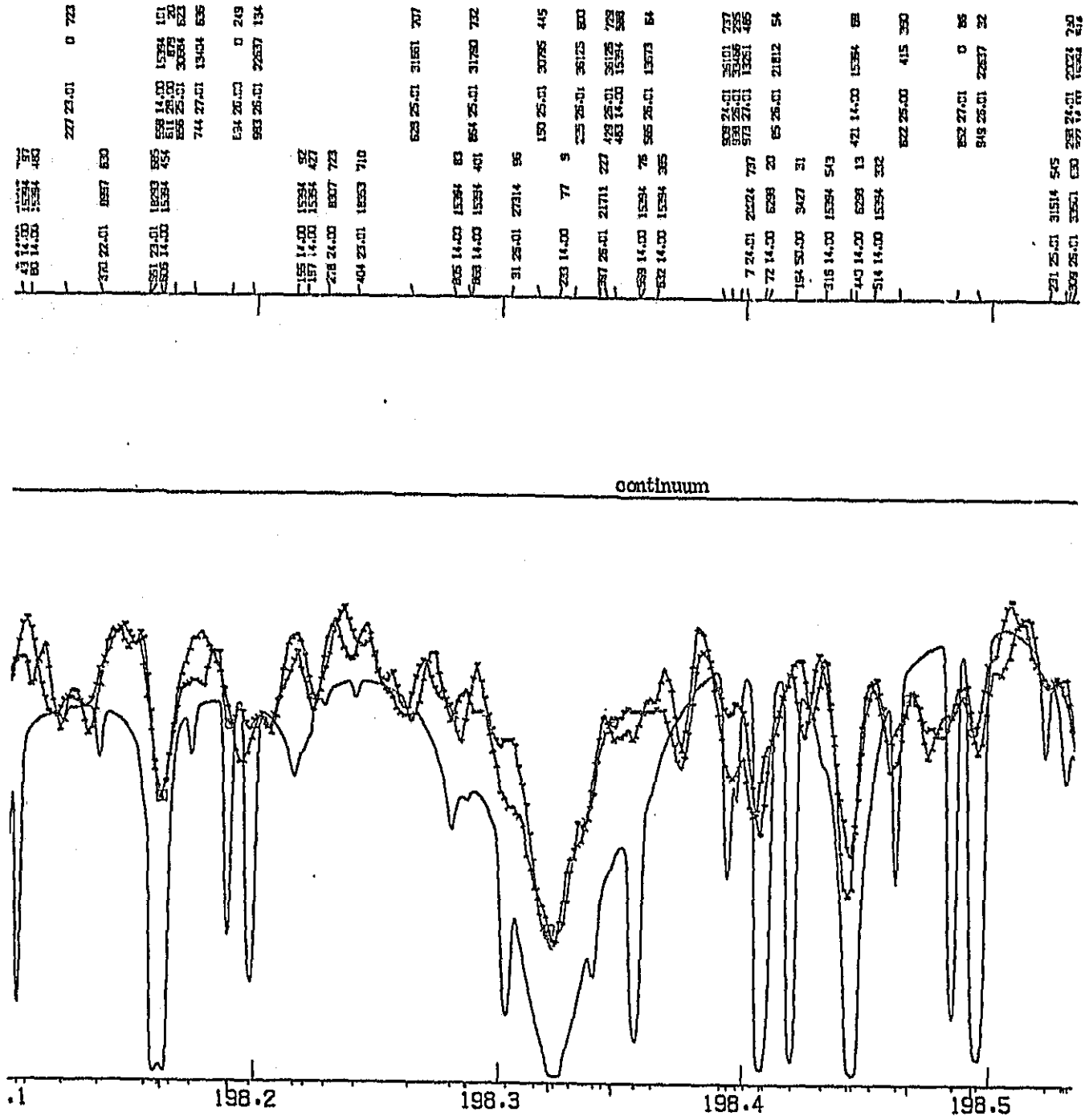

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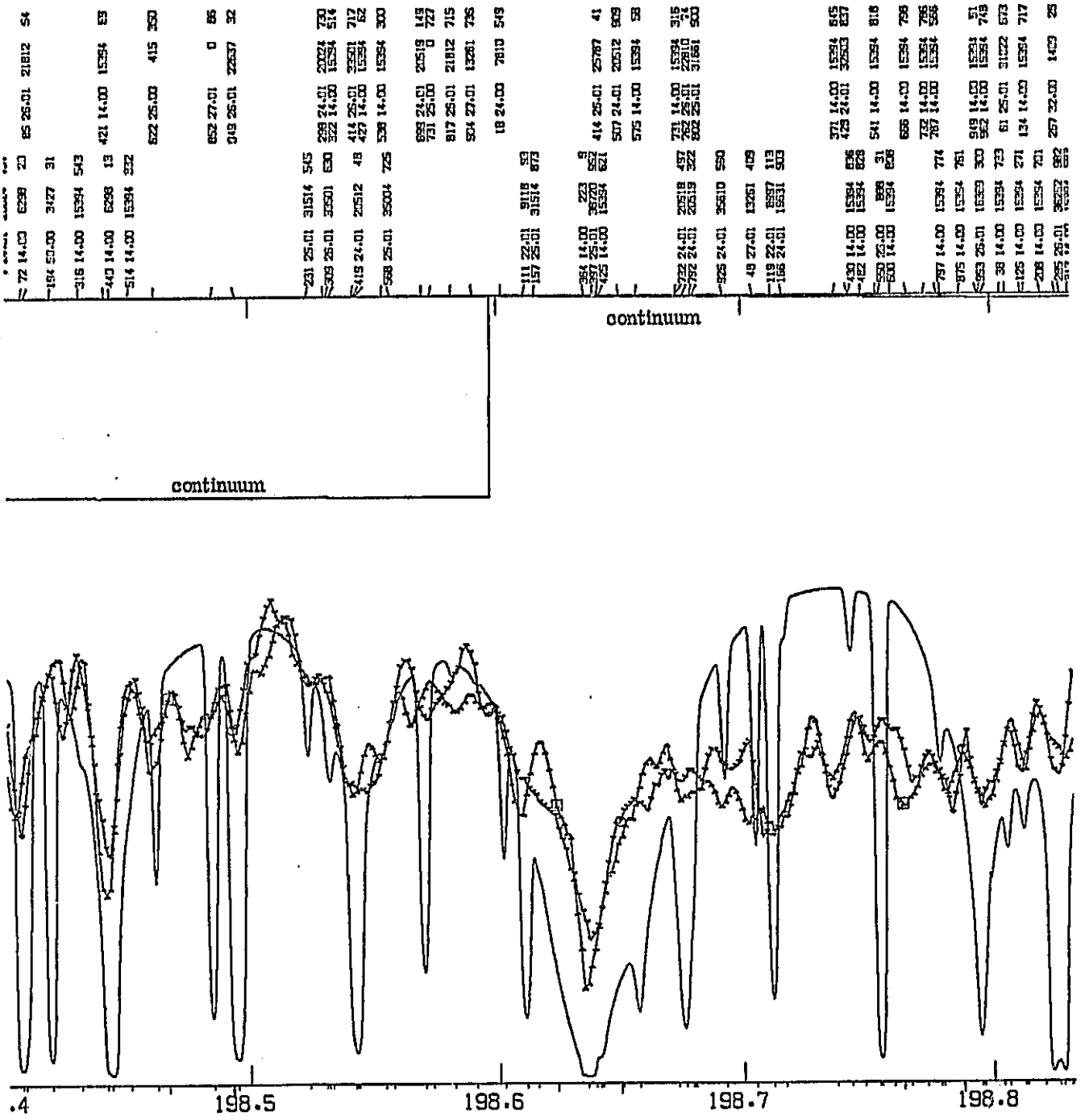

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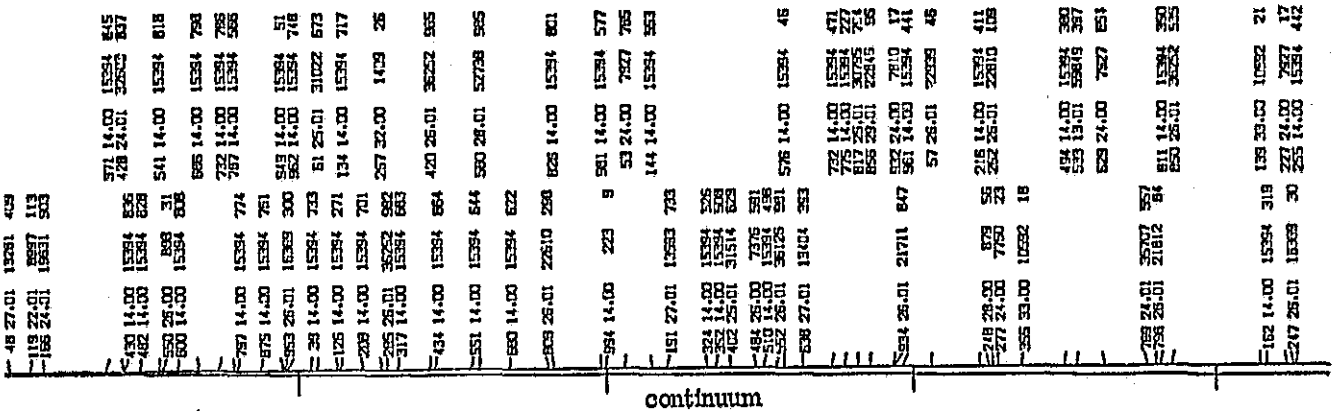

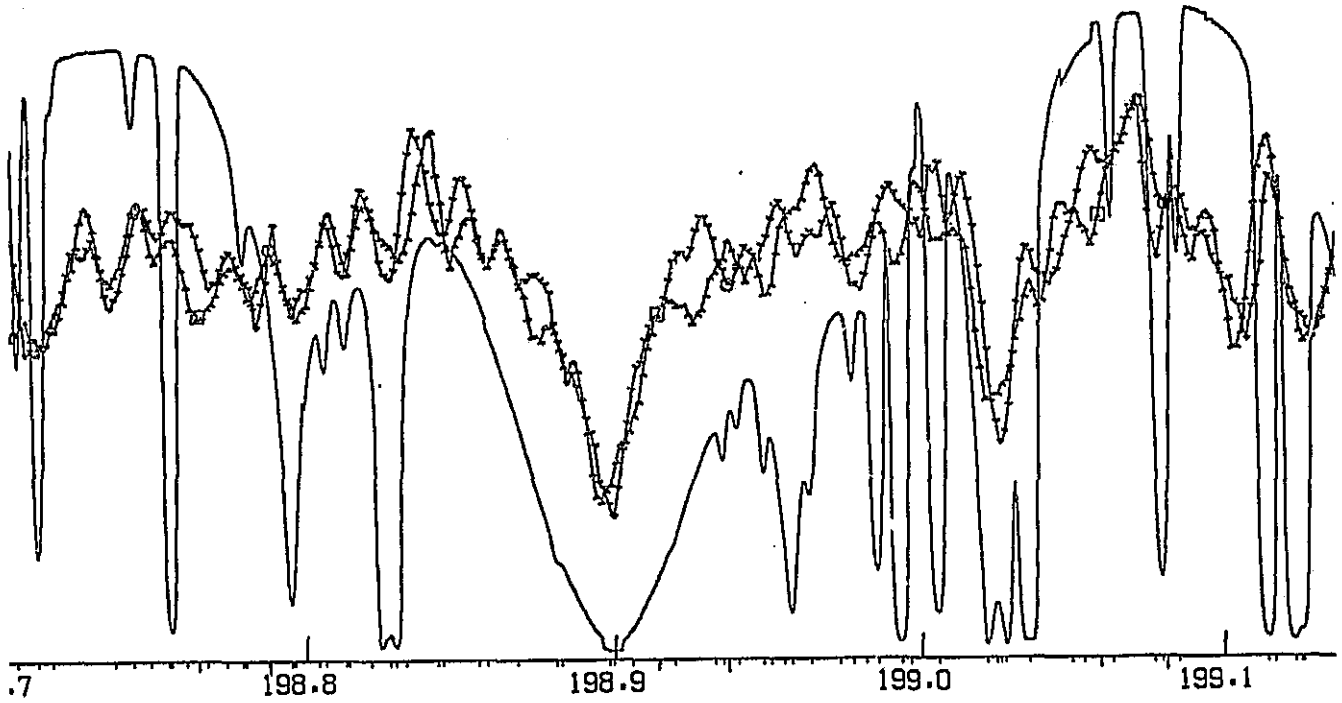

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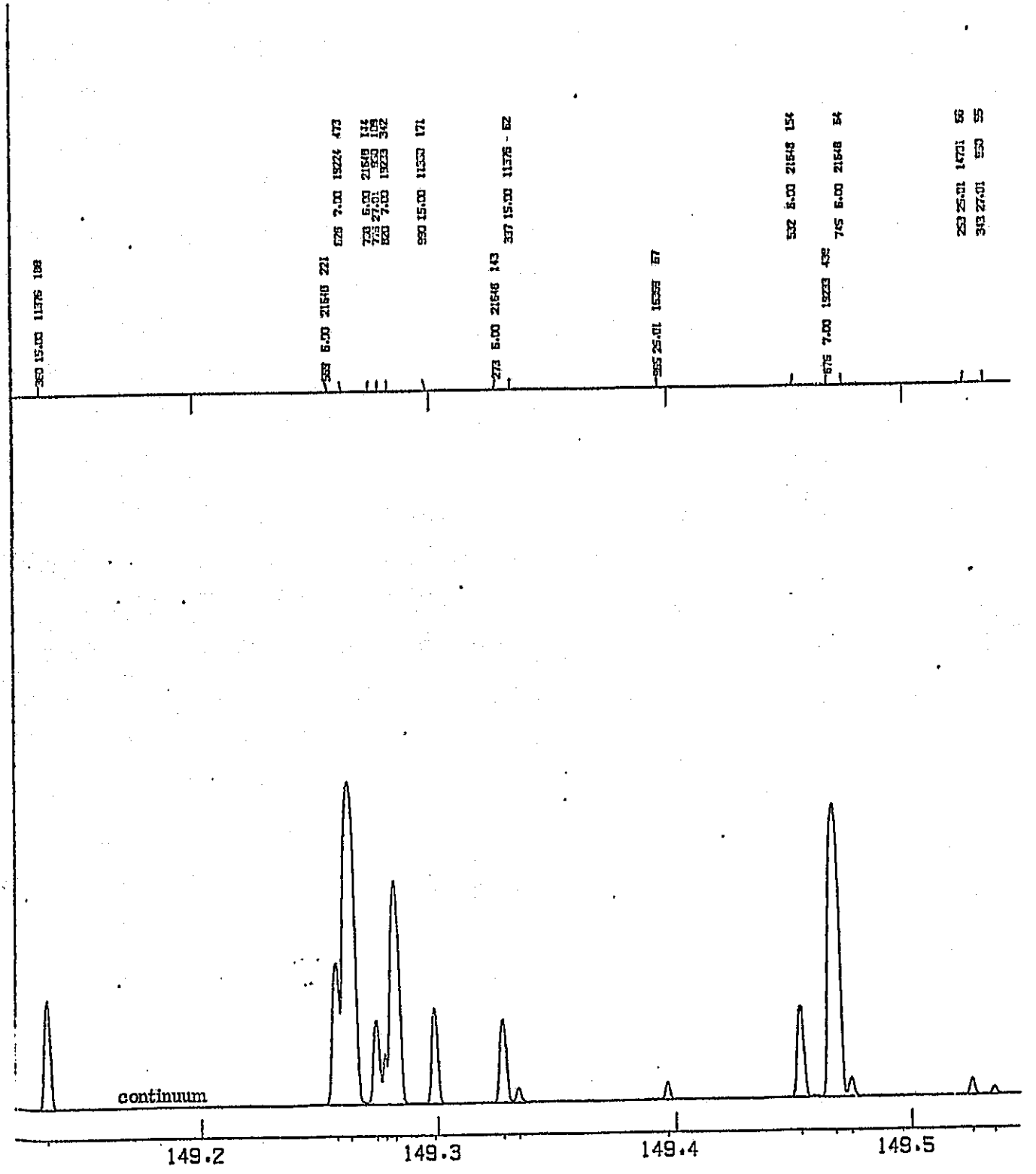

Figure 4. Same as for Figure 3 but for a region showing chromospheric emission lines.

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6. FURTHER WORK

We expect to make a number of improvements over the next two months, then return to NCAR for another iteration on the spectrum. Several problems that we expect to correct are the following.

C II, Mg II, Al II, and Si II lines are computed too weak because they were not based on non-LTE results. Work is underway to calculate departure coefficients for these ions.

Many highly ionized lines do not appear in the calculation. We are adding the coronal approximation to treat such lines.

There are many molecular lines in the observed spectrum. We are adding molecular lines to our line list.

For many lines like Fe II we use an approximate scattering source function in the chromosphere, but emission cores still appear in the calculation, contrary to observation. We are developing a more accurate procedure for dealing with these lines.

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