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# THE CALCULATION OF THEORETICAL CHROMOSPHERIC MODELS AND THE INTERPRETATION OF SOLAR SPECTRA FROM ROCKETS AND SPACECRAFT

NASA Grant NSG-7054

Semiannual Report No. 16 and 17

For the period 1 January 1983 to 30 June 1983
and the period 1 July 1983 to 31 December 1983

Principal Investigator
Eugene H. Avrett

January 1984

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

Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138

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# THE CALCULATION OF THEORETICAL CHROMOSPHERIC MODELS AND THE INTERPRETATION OF SOLAR SPECTRA FROM ROCKETS AND SPACECRAFT

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This year we have made a considerable effort on models and spectra of sunspots because they are important to energy balance and variablity discussions, and yet are poorly understood. We have been fortunate to be able to collaborate with Per Maltby and Olav Kjeldseth Moe of the Institute for Theoretical Astrophysics in Oslo in this research. Kjeldseth Moe is analyzing the sunspot observations in the ultraviolet region 140-168 nm obtained by the NRL High Resolution Telescope and Spectrograph, while Maltby has made extensive photometric observations of sunspot umbrae and penumbrae in 10 channels covering the wavelength region 387-3800 nm. Visits by Avrett to Oslo in August and of Maltby to Cambridge in the fall resulted in basic temperature-density models. Preprints by Avrett and Kurucz, "Photospheric and sunspot models from high-resolution spectrum synthesis", and by Maltby, Albregtsen, Moe, Kurucz, and Avrett "Solar-cycle temperature variations in sunspots", are appended. The next step is a detailed calculation of the spectrum and comparison with observations. The Oslo group is also reducing HRTS data for other solar features and they will make those data available to us.

Kurucz spent January through May at Los Alamos and used time on Cray's, CDC 7600's, and VAXes in a collaborative arrangement for computing cool star opacities and model atmospheres. The sun is the first test case, both to check the opacity calculations against the observed solar spectrum, and to check the purely theoretical model calculation against the observed solar energy distribution. We hope these arrangements will continue in 1984 but we cannot plan into the future because Los Alamos computers are becoming more saturated. Kurucz has not been been able to get access to large computers at any other laboratory. It would be very helpful if there were some way that NASA could provide us with computer time, perhaps at Ames.

Molecules have turned out to be much harder than anticipated and have slowed down everything. Kurucz has been working with Lucio Rossi from Frascati and with John Dragon at Los Alamos. Line lists have finally been completed for all the molecules that are important in computing statistical opacities for energy balance and for radiative rate calculations in the sun (except perhaps for sunspots). These are listed in Table I. Because many of these bands are incompletely analyzed in the laboratory, the energy levels are not well enough known to predict wavelengths accurate for spectrum synthesis and for detailed comparison with observations. Work will continue to improve the quality of the line lists. There are still a number of minor bands to be calculated, such as ultraviolet bands of $C_2$ and CN, and bands of molecular ions. Also, in the infrared, CO is the only vibration-rotation system included at present. We need to add SiO, hydrides, and other molecules as well.

TABLE I

| FILE | NUMBER OF LINES | WAVELENGTH (NM) FIRST | LAST | COMMENT |
|---|---|---|---|---|
| KP | 265587 | 5.2682 | 9997.2746 | Kurucz-Peytremann atomic |
| PREDKP | 696704 | 6.6681 | 9995.4359 | Predicted KP |
| GFFILE | 28420 | 2.4898 | 65101.684 | Additions to KP |
| NLTELINE | 53594 | 22.7838 | 9999.3740 | Can be treated NLTE |
| FE2 | 431933 | 51.2159 | 9988.4949 | Fe II |
| H2 | 28486 | 84.4941 | 184.4573 | Lyman and Werner |
| HYDRIDES | 331268 | 203.6264 | 3245.1715 | CH,NH,OH,MgH,SiH all isotopes |
| CNAX12 | 484709 | 292.5406 | 99912.800 | 12C14N Red |
| CNAX13 | 503631 | 295.1871 | 99924.784 | 13C14N Red |
| CNAX15 | 289887 | 341.5994 | 99776.188 | 12C15N Red |
| CNBX | 323818 | 201.9947 | 715.7552 | CN Violet all isotopes |
| C2AX | 406236 | 271.8071 | 9999.6289 | C2 Phillips all isotopes |
| C2BA12 | 462803 | 389.6061 | 99957.754 | 12C12C Ballik-Ramsay |
| C2BA13 | 387809 | 511.6587 | 99980.746 | 12C13C Ballik-Ramsay |
| C2BA33 | 313319 | 527.1495 | 80319.395 | 13C13C Ballik-Ramsay |
| C2DA12 | 329771 | 344.9621 | 2541.6874 | 12C12C Swan |
| C2DA13 | 253014 | 374.0201 | 991.5625 | 12C13C Swan |
| C2DA33 | 217545 | 376.2757 | 959.4157 | 13C13C Swan |
| C2EA12 | 487232 | 176.0052 | 862.4585 | 12C12C Fox-Herzberg |
| C2EA13 | 332214 | 177.3769 | 560.9010 | 12C13C Fox-Herzberg |
| C2EA33 | 260883 | 178.6938 | 543.2282 | 13C13C Fox-Herzberg |
| COAX | 396004 | 111.3365 | 460.6524 | CO 4th Pos all isotopes |
| COIR | 118920 | 963.5078 | 9998.8853 | CO vib-rot all isotopes |
| SIOAX | 760378 | 177.3128 | 546.2833 | SiO A-X all isotopes |
| SIOEX | 947015 | 143.0468 | 462.4214 | SiO E-X all isotopes |
| TIOAX6 | 325116 | 528.5640 | 1875.4212 | 46Ti16O gamma |
| TIOAX7 | 327496 | 528.7059 | 1771.6149 | 47Ti16O gamma |
| TIOAX8 | 647203 | 490.4263 | 2146.0045 | 48Ti16O gamma |
| TIOAX9 | 332113 | 528.9757 | 1864.4024 | 49Ti16O gamma |
| TIOAX0 | 334222 | 529.1046 | 1860.9887 | 50Ti16O gamma |
| TIOBX6 | 343598 | 246.6118 | 1232.9218 | 46Ti16O gamma' |
| TIOBX7 | 345990 | 246.3570 | 1209.4093 | 47Ti16O gamma' |
| TIOBX8 | 861488 | 235.9828 | 1362.8784 | 48Ti16O gamma' |
| TIOBX9 | 350530 | 246.7795 | 1187.2650 | 49Ti16O gamma' |
| TIOBX0 | 352802 | 247.3491 | 1186.9649 | 50Ti16O gamma' |
| TIOCX6 | 232718 | 350.0947 | 1562.0368 | 46Ti16O alpha |
| TIOCX7 | 234318 | 350.0471 | 1554.5985 | 47Ti16O alpha |
| TIOCX8 | 503950 | 257.0800 | 1316.1735 | 48Ti16O alpha |
| TIOCX9 | 237430 | 350.0113 | 1540.7715 | 49Ti16O alpha |
| TIOCX0 | 238827 | 349.9744 | 1534.3348 | 50Ti16O alpha |
| TIOEX6 | 241398 | 630.6768 | 2002.6215 | 46Ti16O epsilon |
| TIOEX7 | 242954 | 631.0335 | 1997.7022 | 47Ti16O epsilon |
| TIOEX8 | 510074 | 549.4411 | 2273.1493 | 48Ti16O epsilon |
| TIOEX9 | 245978 | 631.7067 | 1988.4477 | 49Ti16O epsilon |
| TIOEX0 | 247466 | 632.0252 | 1984.0965 | 50Ti16O epsilon |
| TIOBA | 310376 | 541.4458 | 2250.2486 | TiO delta all isotopes |
| TIOCA | 223850 | 446.7588 | 1669.0456 | TiO beta all isotopes |
| TIOFA | 153496 | 432.0083 | 816.6252 | TiO f-a all isotopes |
| TIOBD | 158000 | 593.4372 | 2662.9648 | TiO phi all isotopes |
| TIOED | 102107 | 332.9690 | 562.5112 | TiO e-d all isotopes |

As we discuss below, we have discovered that the 1972 Kurucz-Peytremann atomic line data were not able to account for the solar ultraviolet opacity because of missing excited configurations of iron group elements. Generally, laboratory analyses of atomic spectra are not sufficiently complete to predict all the lines that can be significant in the solar spectrum or in computing opacity. In fact, such analyses are often quite inadequate. In order to predict configurations that have not been observed, or that have been only partially observed, and to estimate the configuration interaction among those configurations and the known configurations, it is necessary to make a theoretical calculation. Including these effects also increases the accuracy of the semiempirical calculations for known configurations. In 1972, Kurucz and Peytremann did not have the means to do theoretical calculations and they expected that configurations that had not been seen in the laboratory would not make much difference.

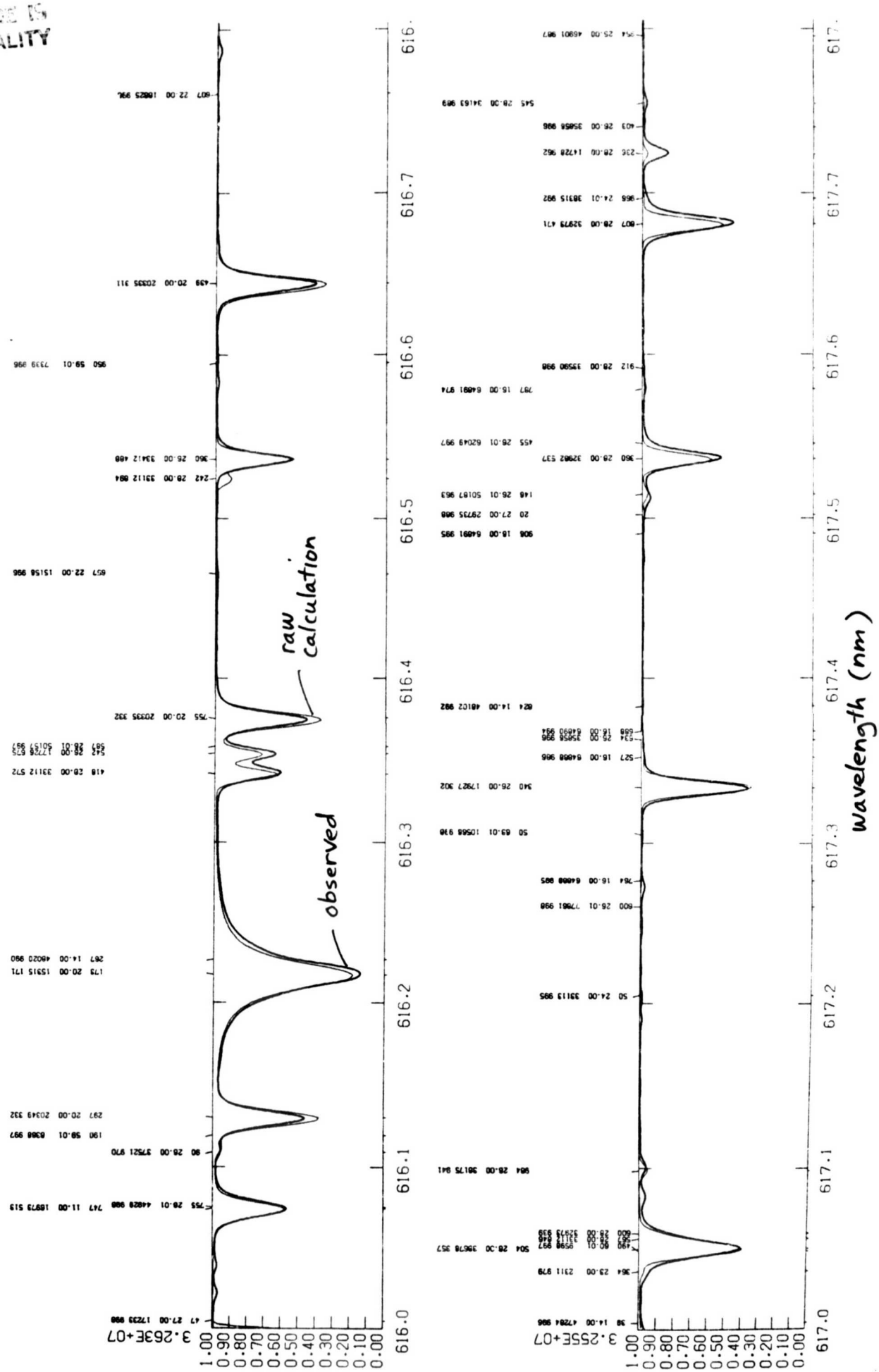
During Kurucz's visits to Los Alamos he has used Robert Cowan's Hartree-Fock program to build up a library of predicted Slater and transition integrals for 50 low configurations of the first 10 ionization stages of the elements up through zinc, and of the first 5 ionization stages for all the heavier elements. These data should quickly allow us to make improved line calculations for the iron group elements that are prominent in the solar ultraviolet. Fe II and Fe I are now being calculated including as many configurations as will fit into our VAX, and with configuration interaction among all the configurations estimated from the Hartree-Fock calculations described above.

The line data listed in Table I were tested by computing spectra from an empirical solar model using the lines with good wavelengths and then comparing to the solar atlases that were available (discussed below). Raw comparisons to uncalibrated spectra in the red and in regions with strong molecular bands were remarkably good as shown in Figures 1 and 2, although we were not able to get a calculation that was completely consistent among all the C bearing molecules and Lambert's abundances. Spectrum comparisons in the rocket ultraviolet still showed many missing lines, but we hoped that they were present in a statistical sense among all our predicted lines. We did not have any spectra with which to test TiO.

Once the line data listed in Table I were ready, Kurucz computed new opacity tables for use in our solar modelling. The calculations involved 17,000,000 lines, 3,500,000 wavelength points, 50 temperatures, and 20 pressures, and took a large amount of computer time. The opacity is tabulated both as 12-step distribution functions for intervals on the order of 1 to 10 nm, and as opacity sampling where, simply, every hundredth wavelength point in the calculation was saved.

As soon as these opacities were completed, they were used to compute a theoretical solar photosphere model, the flux and intensity for the VAL empirical model C, and the intensities for the empirical sunspot model described above. These calculations were performed two ways, once with distribution function opacities and once with the sampled opacities. The calculations were consistent. In Figure 3 we show the the theoretical model irradiance compared to that determined by Neckel and Labs (Solar Physics, 74,231-249,1981), Mount and Rottman (JGR 86, 9193-9198,1981), and Arvesen et al (Applied Optics 8,2215-2232,1969). Molecular bands now show up in the spectrum and there is a general

Fig. 1 – Solar Central Intensity from the Kitt Peak Preliminary Atlas



# Fig. 2 – Solar Central Intensity from the Kitt Peak Preliminary Atlas

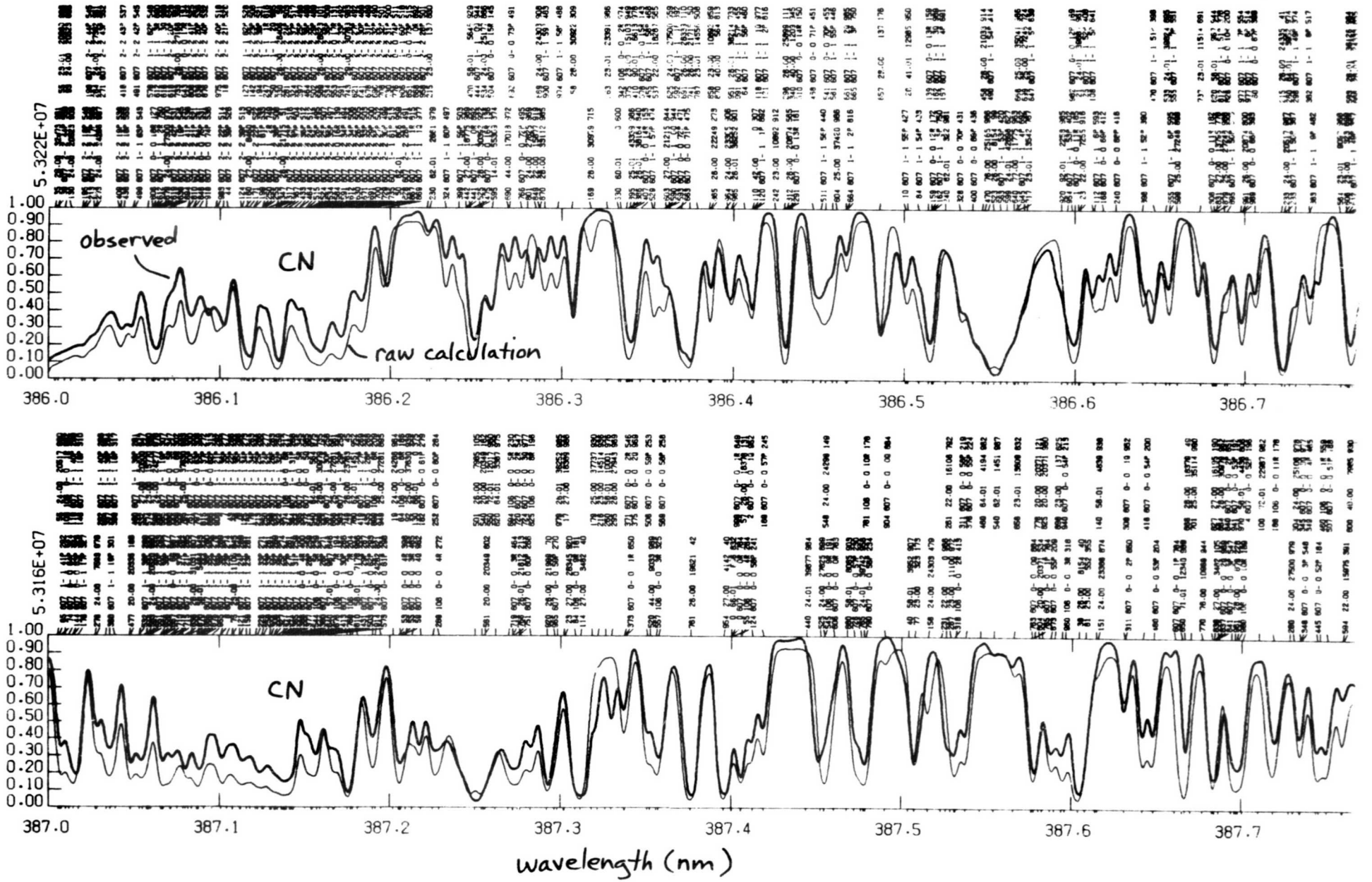
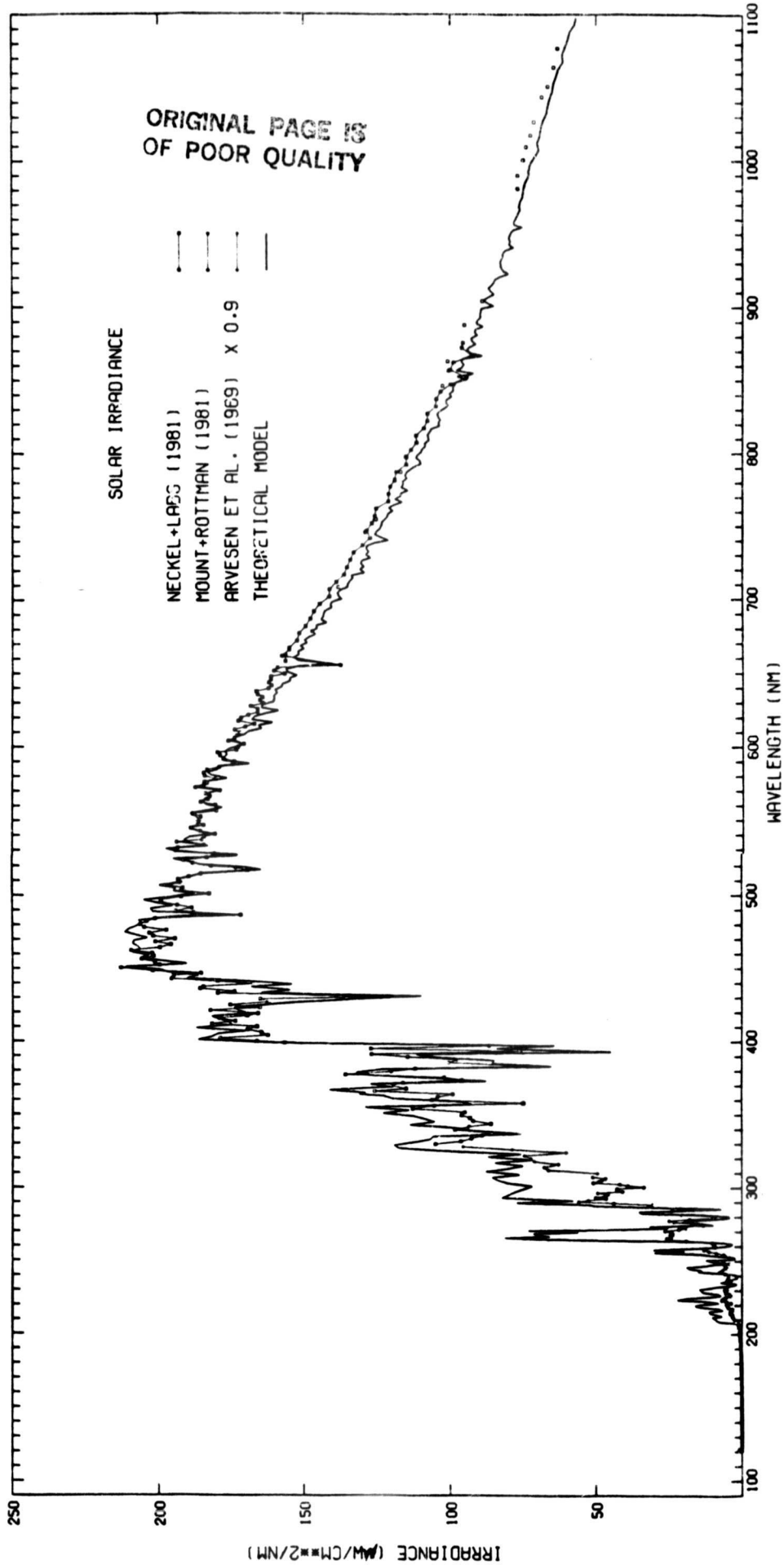


FIG 3


ORIGINAL PAGE IS
OF POOR QUALITY
SOLAR IRRADIANCE
NECKEL+LABS (1981)
MOUNT+ROTTMAN (1981)
ARVESEN ET AL. (1969) X 0.9
THEORETICAL MODEL
IRRADIANCE (MW/CM**2/NM)
WAVELENGTH (NM)
250
200
150
100
50
100
200
300
400
500
600
700
800
900
1000
1100

correspondence of features. Since this is a flux constant model, the integral under both the theoretical and observed curves must be the same. Thus the ultraviolet regions where the flux is too high are balanced by regions in the red and infrared where the flux is too low. These differences were very upsetting because, after all the work on molecules, we had expected a good match, with small differences averaging out. We spent a long time looking for errors in the programs and for physical shortcomings in the convective treatment. These calculations had been done with a new version of Kurucz's model atmosphere program that included horizontal averaging of opacities for convection (Lester, Lane, and Kurucz, Ap.J. 260,272-285,1982). We actually did find some bugs and numerical problems but none of them turned out to be serious. We tried a number of changes in the treatment of convection including writing a new two-component model atmosphere program, but none of the changes made a great difference.

In Figure 4 we show the ultraviolet central intensity computed with VAL model C (Vernazza, Avrett, and Loeser, Ap.J.Supp. 45,635-725) compared to the rocket observations tabulated by VAL (Ap.J.Supp. 30, 1-60,1976, mainly from Kohl et al.). The new calculation is significantly higher than the observed. The VAL models used Kurucz's earlier line opacities but those opacities had to be adjusted to force agreement or near agreement with observation.

We also compared intensities computed from an empirical sunspot model to observations. There seems to be insufficient line opacity all the way through the spectrum even though a tremendous amount of TiO shows up in the visible. These comparisons are somewhat compromised because of Zeeman splitting that is present in the sunspot but not in the calculations. Kurucz is working on a subroutine that will automatically treat Zeeman splitting in detailed spectrum calculations. The new calculations of atomic lines mentioned above will automatically produce g values for all energy levels.

Considering all these problems, and that spectrum comparisons in the ultraviolet still showed many missing lines, we computed, using all the line data, several regions of the spectrum that were most discrepant. (This was quite a feat of tape reading on our VAX.) These spectrum calculations were consistent with the model calculations and showed that at 270 and at 300 nm where the discrepancies were worst, the predicted lines do not account (in the mean) for all the missing lines. We had been expecting that the inclusion of molecular lines would solve all these problems but at these two wavelengths it obviously had not. We next computed a model in which we artificially increased the ultraviolet line opacity and were able to get much better agreement. We then reexamined the Kurucz-Peytremann calculations and concluded that we could find more atomic lines by including higher configurations for the iron-group elements.

We want to emphasize that, although problems remain, we have made tremendous improvements in the treatment of opacity in the course of this work. In Figure 5 we show the predicted continuum level corresponding to the model in Figure 3. The regions that are still giving us trouble have over 80% blocking. We expect to match them in 1984.

Fig. 4



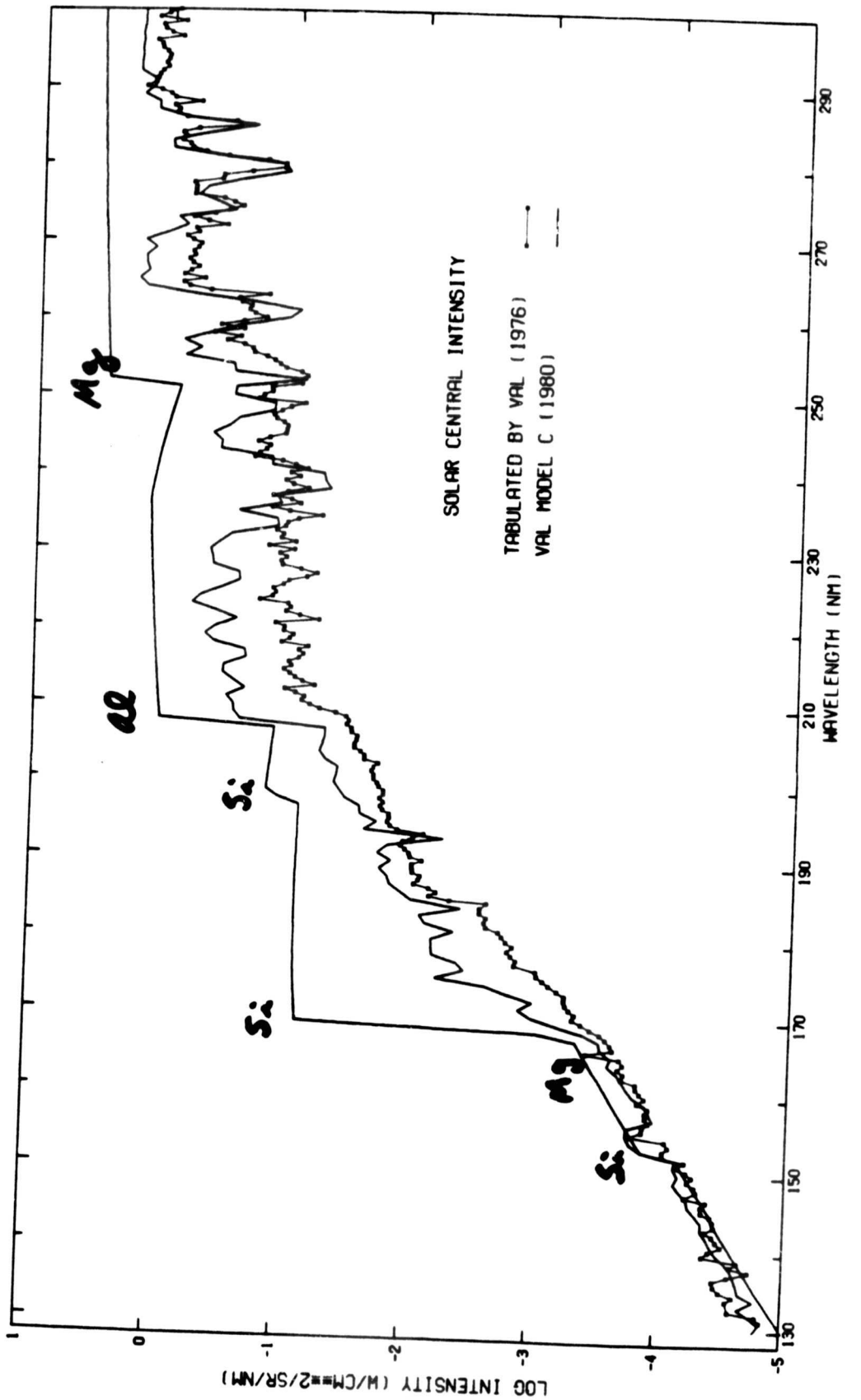
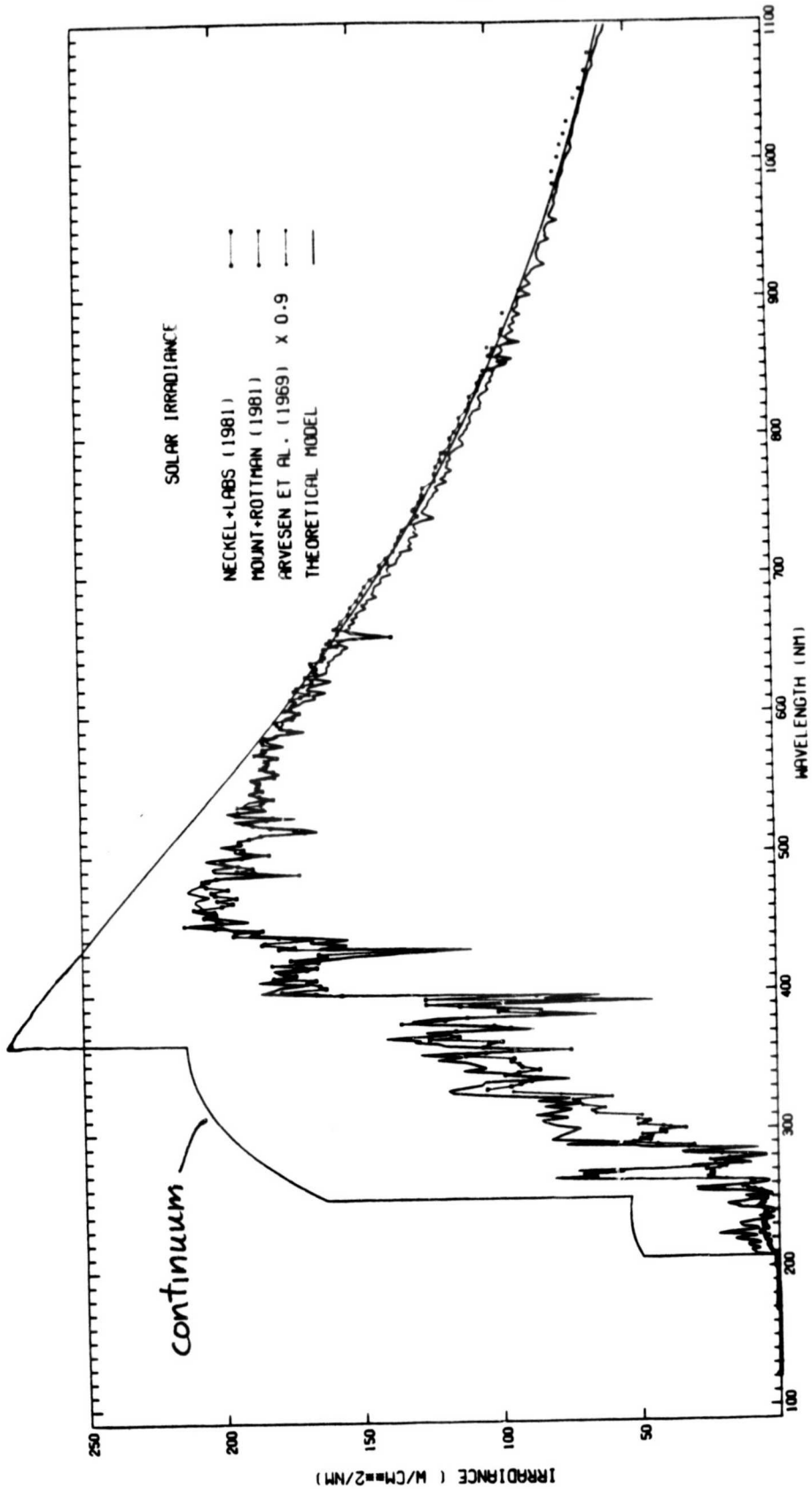


Fig. 5



We also did the following work in 1983.

Peter Ulmschneider asked Kurucz to produce some sort of multifrequency mean opacities for use in acoustic wave chromospheric heating calculations in place of Rosseland means. As part of the opacity calculation Kurucz computed new Rosseland opacities and developed some new types of mean opacities but they have yet to be tested.

Kurucz, Furenlid, Brault, and Testerman have produced an FTS solar flux atlas for 295 to 450 nm with resolution 348000 and signal-to-noise about 8000, and for 450 to 1300 nm with resolution 521000 and signal-to-noise about 4000. The atlas is plotted as pseudo-residual flux with a conversion factor to the Neckel and Labs (Solar Physics, 74,231-249,1981) absolute calibration. We are now trying to obtain funding for publication. This atlas has been invaluable in testing our line data.

We needed sunspot spectra for comparison with our calculations. Engvold has kindly given us access to his FTS observations of sunspots and nearby disk. Kurucz reduced these following the same procedures that he used for the solar flux atlas. Kurucz has synthesized spectra for Maltby's 10 bandpasses and compared to Engvold's spectra. There are considerable discrepancies that we are trying to understand.

We obtained, and are using in spectrum synthesis comparisons, the Delbouille, Roland, Brault, and Testerman solar intensity atlas for 1 to 5 micrometers. With the help of Larry Testerman we have also obtained FTS data from Kitt Peak for 8-13 micrometers, and we also have data from Goldman et al at Denver for the far IR but they are not yet usable. We have had no time this year to improve our treatment of atmospheric transmission which is important in using these atlases. Kurucz has made no progress on reducing OSO8 or Harvard rocket or UVSP spectra this year.

John Dragon of Los Alamos has been studying solar ultraviolet opacity for a long time. He used some of Kurucz's data and programs in his thesis. He has decided that he has to be able to do rigorous non-LTE radiative transfer in order to make further progress. Dragon has been combining the Auer and Mihalas programs (with their help) with Kurucz's non-LTE opacity and molecular equilibrium programs and line data (with Kurucz's help). Dragon expects to produce an alternative to Pandora with which he can check our calculations. The program at Los Alamos is being developed on the Cray and we will get a copy once it is working. Right now we are limited to running Pandora on the VAX which is very slow. With access to a Cray we will be able to do much more extensive calculations.

Larry Petro, Warren Rosen, and Peter Foukal have been searching for solar limbdarkening variations that presumably would reflect changes in the structure of the solar atmosphere from changes in convective efficiency (Petro, Foukal, Rosen, Kurucz, and Pierce submitted to Ap.J.). Kurucz is collaborating with them and has the responsibility for finding mechanisms and theoretical derivatives for such variations. Unfortunately our old models do not reproduce the solar limbdarkening and do not include the molecular opacity that would be the most sensitive component to the variation. Our new model does have the molecules but it still is not right. We hope that our next try at the opacities will finally do the job.