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AN ANALYSIS BY WAVELENGTH COINCIDENCE STATISTICS OF THE ULTRAVIOLET SPECTRUM OF KAPPA CANCRI

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ABSTRACT

IUE wavelengths in the mercury-manganese star κ Cnc have been analyzed using the method of wavelength coincidence statistics. The method has been adapted to include line intensities for the second and third spectra of iron and manganese, which were calculated for a temperature of 12,600 K with the help of the Kurucz-Peytremann transition probabilities. This method would clearly benefit from improved basic atomic data, both for wavelengths and for transition probabilities.

Using a slab (Schuster-Schwarzschild) model, we have investigated the level of ionization of iron and manganese from single to doubly ionized stages, and find agreement with LTE predictions within what we consider the accuracy of the method—0.3 to 0.5 dex. Relative numbers of doubly ionized iron and manganese atoms have been estimated, and are found to be equal, within our uncertainties. We conclude that the large manganese excesses for κ Cnc ($\sim$2 dex), which have been based primarily on the trace species Mn^+, cannot be attributed wholly to non-LTE or to the concentration of manganese into a cool, thin layer. If these effects are present, they are at the level of our errors.

Subject headings: stars: abundances — stars: peculiar A — stars: individual — ultraviolet: spectra

I. INTRODUCTION

Stellar spectra obtained with the *International Ultraviolet Explorer* (*IUE*) are difficult to analyze. Most users are familiar with the problems of wavelength and intensity calibrations as well as noise. In addition to these matters, there are difficulties which arise from the nature of atomic spectra and their current state of analysis. A canonical figure for the fraction of unidentifiable features in the ultraviolet is 50% (Kurucz and Avrett 1981).

The line densities of the first and second spectra of the ubiquitous iron-group elements are typically at their maxima in the region of the *IUE* spectra, and it is not difficult to show (Cowley 1981) that many lines are expected from levels that have not yet been identified by laboratory studies.

The general situation with regard to the analysis of *IUE* spectra is quite similar to that which faced the student of the ground-based spectra of the more extreme magnetic Ap stars. For these objects, the method of wavelength coincidence statistics (WCS) has been shown to be a useful tool. We shall not review the technique here (see Cowley and Hensberge 1981; Wolff 1983, and references cited therein). The chief advantage of WCS over traditional methods which attempt to identify individual features is that "misidentifications" occur only in a statistically predictable sense. When one identifies a species at a given confidence level, the line density, including the unidentifiable features, is taken into account explicitly.

A few recent studies have made use of WCS *in addition to* traditional methods. Bord and Davidson (1982) analyzed *IUE* spectra, while Van Santvoort and Hensberge (1981) used BUSS data. However, up to now, line intensities have played only a minor role in the WCS procedure; a primary purpose of the present study is to add this dimension.

Laboratory intensities have several disadvantages which make them of limited value in "advanced" line identification studies. The conditions in the laboratory source may be quite far from those in the stellar atmosphere. Indeed, intensities from the commonly used nonthermal sources can be counterproductive. Use of relative intensities within multiplets is the traditional palliative for this problem. It works well in rudimentary identification studies, but in more advanced applications various complications encumber the paradigm procedures. *LS*-coupling multiplets are often a poor description of the real atomic spectrum. Moreover, when one line in two cannot be safely identified, the relative intensities, even in well-defined multiplets, can be distorted to the point where the multiplet may no longer be recognized.

These are not valid arguments for *ignoring* laboratory intensities. They do provide a motivation for seeking more satisfactory sources of intensity. When oscillator strengths are known, one can in principle produce a list of relative intensities that should be relevant for any thermal source. This is the approach taken in the present work. The inevitable nonlinearities due to curve-of-growth effects are, for the present, accepted. We adopt the Kurucz-Peytremann (1975, KP) tabulation as the source of our oscillator strengths. At this time, there is no reasonable alternative reference that could provide the large number of transition probabilities needed for the current study. We shall address the question of the inaccuracies of the *gf-values* and their influence on our results below.

As an initial problem, we have chosen to analyze the Fe II, Fe III, Mn II, and Mn III spectra in the *IUE* wavelengths of the mercury-manganese star κ Cnc. The stellar measurements consist of 4548 wavelengths in the region $\lambda\lambda$1223–2097 (SWP), and 2524 in the region $\lambda\lambda$1969–3227 (LWR). The LWR measurements were described by Bord and Davidson (1982). Essentially the same technique was followed to produce the SWP set.

It is of interest to intercompare the second and third spectra of iron and manganese in κ Cnc because of conflicting results from abundance studies for these elements (see Table 1) as well as the possibility of element stratification which, according to the work of Alecian and Michaud (1981) and Alecian (1982),

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TABLE 1

RECENT MANGANESE AND IRON ABUNDANCES FOR κ CANCRI log $(H) = 12.0$

Reference	Mn	Fe	T_e	log (g)	ξ_t
Guthrie 1984	7.2	7.8	13500	3.65	3
Heacox 1979	9.3	8.5	13500	4.0	0
Heacox 1979	8.5	7.9	13500	4.0	3
Kodaira and Takada 1978	7.2	7.6	14400	3.6	3.2
Allen 1977	...	7.7	13700	3.7	0
Dworetsky 1971	7.8	7.8	14000	3.6	5

could lead to the concentration of the manganese atoms in a relatively thin layer high in the stellar photosphere.

There is an additional point which deserves to be mentioned here, and that is the validity of an LTE analysis in a description of the stellar spectrum. The observational results for Mn II in the classical mercury-manganese stars have been well described by Wolff and Preston (1978, see their Fig. 2). The Mn II lines become typically stronger, the *higher* the effective temperature of the star. Classical theory would lead one to suspect that the Mn II lines would weaken—a simple calculation shows that there should be about equal numbers of singly and doubly ionized manganese atoms close to an effective temperature of 11,000 K, which is near the low-temperature boundary of the mercury-manganese stars.

Thus standard LTE analyses have yielded abundances which were an increasing function of the stellar effective temperature (Aller 1970; Wolff 1983). An alternate possibility, that the Saha equation leads to an overestimate of the degree of ionization of manganese, has not received much attention.

II. METHOD: ASSUMPTIONS AND PROCEDURES

We assume that a list of intensity estimates for each atomic line can be generated from the KP tables. In practice, we have calculated an estimate for the logarithm of an intensity parameter, IP, using the relation

$$\log(\mathrm{IP}) = \log(gf) - \theta\chi\,. \tag{1}$$

We have used $\theta = 0.4$ in the present study, corresponding to a temperature of 12,600 K.

In the simplest application of our procedures, we make a table of wavelengths and intensities for Fe II lines, for example, within some wavelength region covered by the stellar measurements. The table is then sorted according to the intensity parameter, and WCS trials are run starting with the n strongest lines, the next n strongest lines, etc. In a typical run for Fe II or III, we used $n = 100$. The strongest set of lines yield identifications with high confidence levels, and the significance parameters diminish as the average intensities of the sets decreases. An example is shown in Figure 1. The S-parameter is defined by

$$S = (H - \langle H \rangle)/\sigma\,, \tag{2}$$

where H is the number of coincidences or hits on the laboratory wavelengths, and $\langle H \rangle$ is the average number of hits on 200 sets of n nonsense or control wavelengths. The parameter σ is the standard deviation of the coincidences on the nonsense wavelengths.

The uncertainties in these S-parameters will be of interest. They will be different for every set of laboratory and stellar lines, so that it is impractical to do more than provide an estimate of the uncertainty in S. We have done this for a few sample cases, using repeated runs with the same atomic line lists, but generating the random numbers for the nonsense lines using a "seed" whose value depends on a sampling of the clock. The results are shown in Table 2. Three different sets of Fe III lines were used. All results are based on 200 sets of nonsense wavelengths.

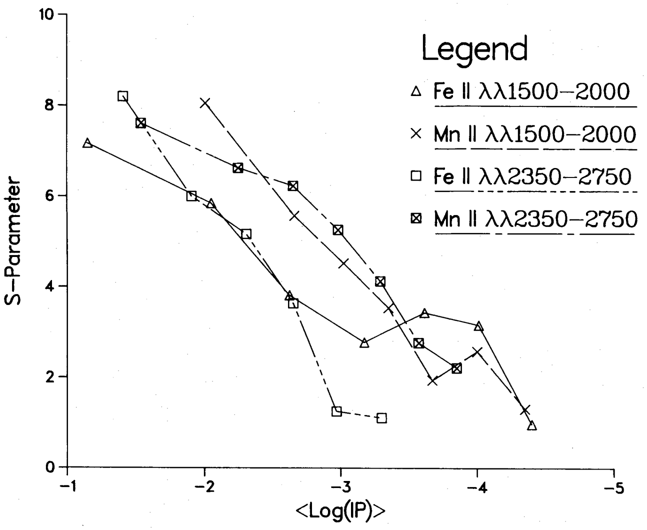

FIG. 1.—WCS tests with atomic spectra and wavelength intervals as noted in the legend. The S-parameter (a measure of the presence and strength of a set of lines) vs. the average logarithm of an intensity parameter (see text). Each point for a given species refers to a set of 100 lines.

The S-parameters seem rather well determined, but it is likely that the smaller values are less secure than the larger ones. Especially near threshold (S values of 2 to 3), S tends to jump around. The most likely explanation of this is errors in the oscillator strengths. It is well known that certain of the KP gf-values are underestimated by orders of magnitude because of atomic interactions that could not be properly taken into account. If enough of the underestimates occur in a given sample of lines, the significance parameters will be distorted. The WCS parameters will still indicate that the lines are present in the spectrum, when one would no longer expect this, because of the (spuriously) low intensity parameters. There is virtually no way to avoid this effect, but we have tried to minimize it in the present work by giving more weight to the results obtained with the higher S-parameters. These are less likely to be changed by a few erroneous gf-values than the borderline cases, where a small number of errors could push the significance parameters from below our threshold (95% confidence) into the category we consider to be "marginally" significant (95%–99.5% confidence).

TABLE 2

SUCCESSIVE ESTIMATES OF THE S-PARAMETER

Fe III 50 lines	Fe III 50 lines	Fe III 50 lines	Mn III 100 lines
2.93	4.14	1.67	3.78
2.65	4.02	1.59	3.65
2.76	4.34	1.61	3.86
3.10		1.80	3.71
2.81		1.58	3.47
2.64		1.64	3.75
			3.86

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It is entirely possible that the KP calculations could be systematically in error for one atomic spectrum vis-à-vis another. It would be very difficult for us to evaluate this possibility at the present time. Only an improved set of calculations would allow us to do this properly, and our present efforts emphasize the need for such work.

There is another source of systematic error that can perturb a study of the present kind. We have assumed that the accuracy of the atomic wavelengths for all of the species is comparable. This is probably not the case. We note that Kurucz and Peytremann cite Edlén's (1973) review as the basic reference for energy-level data. While the sources given by Edlén are still current in our wavelength domain (cf. Corliss and Sugar 1977, 1982), there is an intrinsic problem in measuring the wavelengths of manganese, due to the hyperfine structure, that does not similarly affect wavelengths for iron. We have made a spot check of 30 to 40 wavelengths in the range λλ1000–3000 in the KP tabulation with those listed by Reader and Corliss (1980), for the four relevant spectra. The standard deviations (Reader and Corliss minus KP) are 0.014 Å for Mn II, 0.013 Å for Mn III, 0.013 Å for Fe II, and 0.007 Å for Fe III.

We have attempted to simulate such wavelength errors by adding Gaussian random numbers to our basic laboratory sets. The random numbers had zero means and standard deviations of 0.01 Å, 0.02 Å, etc. We describe these random numbers as Gaussian (0, 0.01), (0, 0.02), etc. With the 100 *unperturbed*, KP, Mn III wavelengths we obtained an S parameter of 5.2. Adding a Gaussian random number (0, 0.01) to each of the 100 wavelengths, and running the WCS test again, we obtained an S parameter of 4.5. Trials adding the random number sets (0, 0.02), (0, 0.03), and (0, 0.04) resulted in S parameters of 3.6, 3.3, and 3.4, respectively.

These results show that the wavelength accuracy is an important matter. If we look at the spectra of the dominant species, the Fe III wavelengths are more consistent than those of Mn III. However, it is not necessarily true that the laboratory wavelengths for Mn III are better, for our purposes, than those in KP. The KP wavelengths were derived from the tabulated energy levels, which typically depend on several wavelength measurements. Consequently, it is possible that the KP wavelengths may actually be better than the original laboratory measurements. A decision cannot be made in the absence of a superior system of measurements. We are again in the position of requiring better fundamental atomic data.

Two additional sources of systematic effects could influence the WCS. Hyperfine structure might actually enhance the visibility of lines in the stellar spectrum. This could mean a bias in favor of Mn II and III. An additional bias might result from the fact that the stellar wavelength scale was based primarily on the identification of iron lines. A proper investigation of these effects by means of a simulation would involve very elaborate calculations that are beyond the scope of the present investigation.

After due consideration, we have decided not to attempt any quantitative adjustments for these systematic effects beyond the admission of a liberal uncertainty in the estimated abundance ratios (~ 0.5 dex).

If the systematic errors are neglected, we may interpret marginal significances, 95 to 99.5% confidences, with S of the order of 2 to 3, as belonging to lines whose strengths were at the threshold for measurement. In a simple spectrum, such as the ground-based photographic spectrum of κ Cnc, we can easily estimate what this threshold is. It is more difficult in the satellite ultraviolet, where the blending is so much more severe. Nevertheless, we may assume that whatever this strength is, it will be the same for two sets of lines with significance parameters at threshold, provided the range *and* distribution of the wavelengths is the same in the two sets of atomic lines. Similar arguments apply to any significance level, provided we ignore non linearities analogous to differential curve-of-growth effects.

These considerations allow us to make crude, slab-model estimates of the ratios of the number of ions present in the photosphere. For any two line lists, chosen as indicated above, we assume equal values of

$$\langle \log (gf) - \theta\chi \rangle + \log (N_r/u_r) \equiv \langle \log (\mathrm{IP}) \rangle + \log (N_r/u_r) , \quad (3)$$

assuming equal values of the statistical parameters. N_r is the number density of atoms in a given ionization stage including all excitations. The angular brackets around the log $(gf) - \theta\chi$ indicate that it is an average for the line list. The quantity u_r is the partition function for the species in question. We assume the equivalent width or central depth of a line is a monotonic function of the probability that the line will be measured. The simple arguments leading to equation (3) for a single line are given by Cowley (1970, see eqn. 2-9.2 and 4-4.1).

If we are to have a meaningful comparison of two sets of WCS parameters for laboratory lines, it is important that the stellar wavelength regions within which the laboratory lines are compared be either the same or closely comparable in every respect. If two sets of atomic lines are chosen on the basis of their intensities, they are unlikely to have the same wavelength distribution, and the direct comparison of the WCS will have a bias.

When one has a very large number of atomic lines, as in the case of Fe II and Mn II, it is possible to avoid this difficulty. But for Mn III, only the strongest 100 lines give convincing WCS parameters. This is true for both the LWR and SWP wavelength ranges. There were many more Fe III lines in the KP tables, so we were able to match closely the intensity and wavelength coverage of the strongest sets (SWP and LWR domains) of the Mn III lines. This match was made with the help of sort and edit routines that were tedious to apply. It might be useful to automate this procedure in future work.

For most of our comparisons, we restricted the range of stellar wavelengths as a palliative to the variable line density. We did not take explicit account of wavelength gaps in the *IUE* measurements which result from the echelle orders. Some bias may be introduced by these gaps, but the effect will be minimized when there is an equal chance that laboratory and nonsense wavelengths can fall within them, as was the case.

Equation (3) leads directly to the following estimate for the logarithmic ratio of number densities of a "primed" and "unprimed" species:

$$\log (N_r'/N_r) = \langle \log (\mathrm{IP}) \rangle - \langle \log (\mathrm{IP})' \rangle + \log (u_r'/u_r) . \quad (4)$$

It is instructive to compare results from equation (4) with the predictions of the Saha equation as well as previous abundance calculations. In order to do this we have to choose a "representative" slab from a model atmosphere tabulation. We find the logarithmic ratios for doubly to singly ionized species shown in Table 3 for two Kurucz (1979) models with abundances enhanced by 0.5 dex. Temperatures and electron pressures were taken from log $(\tau_{5000}) = 0.2$. If we may neglect the effects of blanketing by overlapping lines, the *continuous*

TABLE 3

LOGARITHMIC RATIOS OF SECOND TO FIRST IONIZED SPECIES FROM THE SAHA EQUATION

T_e (K)	Iron	Manganese
13,000.........	0.70	0.96
14,000.........	1.12	1.37

TABLE 4

S-PARAMETERS OF Mn III

	λλ1500–2000		λλ1980–2480	
TRIAL	100	50	100	50
1.........	5.45	5.17	2.49	2.59
2.........	0.95	2.15	−0.95	1.34

opacity at λ5000 should be within a factor of 2 of the opacity in the range λλ1500–2200, which is of interest to us.

At $T = 12{,}600$ K, log [u(Mn III)] = 0.95, log [u(Mn II)] = 1.31, log [u(Fe III)] = 1.52, and log [u(Fe II)] = 1.92. We have used these values for both temperatures of Table 3, as well as in the calculations below. The errors so introduced are negligible in the present context.

III. RESULTS AND CONCLUSIONS

We have obtained WCS parameters for a large number of laboratory line lists for the four atomic species with which we have been concerned. Only a representative sample of the results will be reported here. Figure 1 is a plot of the S-parameter versus the mean value of log (IP) for Fe II and Mn II lines. If we subtract the values of ⟨log (IP)⟩ for Mn and Fe at $S = 4$, we obtain 0.7 dex for the λλ1500–2000 set and 0.8 dex for the λλ2350–2750 set. These differences are subject to the choice of the level of S at which they are taken. We believe both the lowest and highest values are to be avoided. In any case, the uncertainties must be *at least* 0.3 dex, so the very good agreement between the two wavelength regions is fortuitous. If these results are inserted into equation (4), we find roughly equal number densities of singly ionized iron and manganese atoms (0.1–0.2 dex for the logarithmic ratio).

The third spectra have been more difficult to analyze. There are many more Fe III lines than Mn III lines, and only the strongest Mn III lines yield S-parameters over 4.

We shall discuss results for Fe III first, since the statistics for this ion are better defined than those for Mn III. S-parameters for Fe III are compared with those for Fe II in Figure 2. The wavelength region was λλ1980–2480 for both ions. Results for the LWR stellar wavelength set are chosen because the line density is a weak function of wavelength. It was necessary to use only the shortest wavelength portion of this list, because at longer wavelengths there were not enough strong Fe III lines. The 100 strongest Fe III lines in λλ2350–2750, for example, failed to give a significant number of coincidences.

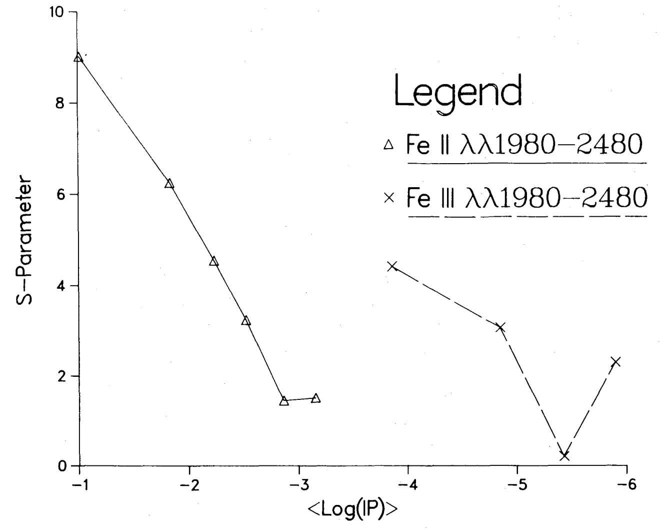

FIG. 2.—See caption to Fig. 1

At the $S = 4.0$ level, the differences in the log (IP) values for Fe II and III is approximately 1.85 dex. Equation (4) then gives 1.45 dex for log (Fe^{++}/Fe^{+}). The expected value, from Table 3, is between 0.7 and 1.1 dex, so the "observed value" is a factor of 2 or 3 higher. This should probably be considered to be agreement within the uncertainties of the technique. The important point is that the ionization does not appear to be discordant by an order of magnitude or more.

Table 4 gives the results of tests with Mn III lines using two SWP and two LWR stellar line sets. For each of the two stellar domains, we performed WCS tests with the n strongest lines, the "next" n strongest, and so on. The table presents results where n is 50 and 100. The wavelengths used in trials 1 and 2 in the $n = 50$ columns are the same lines used in trial 1 in the $n = 100$ columns. Often, when the intrinsic intensitites of the laboratory wavelengths vary in relatively large increments from the strongest to the weakest, it is most fruitful to search for only the very strongest lines. Whether this is in fact true depends upon several factors, such as the strength of the atomic line spectrum under consideration in the stellar spectrum, and the density of stellar wavelengths. When this line density is high, high significance levels can be reached only when coincidences are found in a large fraction of a relatively long list of laboratory lines.

Table 4 shows that significance can be lost by extracting the 50 strongest lines out of the top 100. This is probably due to the high stellar line density. The large values of S, such as those shown in Figure 1, result from trials where some 70 or more coincidences out of 100 were found.

The 100 strongest Mn III lines yielded an S parameter of 2.49 in λλ1980–2480, and since the Mn III lines become even weaker toward longer wavelengths, it has been necessary to use the SWP measurements if values ≥4.0 are to be obtained.

Table 5 gives the relevant data for the determination of the degree of ionization of manganese. The atomic line sets were limited to the domain λλ1500–2000, and contained 100 lines. The data for Mn II have been plotted in Figure 1. If a similar

TABLE 5

S-PARAMETERS FOR Mn II AND Mn III LINES

LINE SET	Mn II			Mn III		
	S	⟨log (IP)⟩	⟨λ⟩	S	⟨log (IP)⟩	⟨λ⟩
1.........	8.18	−2.01	1852	5.45	−4.51	1908
2.........	5.64	−2.68	1846	0.95	−5.17	1824
3.........	4.70	−3.05	1849			
4.........	4.07	−3.38	1851			
5.........	2.32	−3.70	1850			

plot is made, including the Mn III data, we find for the $S = 4$ level a difference in the $\langle \log(\mathrm{IP}) \rangle$ values of 1.5, and this implies $\log(\mathrm{Mn}^{++}/\mathrm{Mn}^{+}) = 1.1$.

From Table 3, we would expect about 1.2 for this number, so, as with iron, the empirical results from WCS appear to be in good accord with the slab-model estimate.

The most important of all comparisons is that for Mn III and Fe III, since these are spectra from the dominant ions, and their relative strengths will give us the abundance ratio independent of all but the most egregious departures from ionization equilibrium. Unfortunately, this particular comparison has been the most difficult for us to determine.

If we simply draw the S versus $\langle \log(\mathrm{IP}) \rangle$ curve for Mn III and Fe III, they fall rather closely on top of one another, and this would give, by equation (4), $\log(\mathrm{Fe}^{++}/\mathrm{Mn}^{++}) = \log[u(\mathrm{Fe\ III})/u(\mathrm{Mn\ III})] = +0.57$. This result seemed rather large to us. One possible way to disqualify it is to look at the distribution of wavelengths, which is a little different for any of the two sets. We have spent some time carefully editing Fe III wavelengths in an attempt to mimic that of the Mn III lines. The results of WCS for the "edited" Fe III lines were S-parameters *smaller* than those for the Mn III lines with comparable values of log (IP). The results of one such comparison are shown in Table 6.

These results may not be directly compared unless we make some estimates for the slope of the S-parameter versus $\langle \log(\mathrm{IP}) \rangle$. From the graphs that we have plotted, we may estimate that $\Delta\langle \log(\mathrm{IP}) \rangle/\Delta S$ is roughly in the range 0.17–0.33. The difference in the S-parameters of Table 6 of $5.45 - 3.63 = 1.82$ implies a difference in the $\langle \log(\mathrm{IP}) \rangle$'s of 0.31–0.60. If we put 0.45 on the right of equation (4), we find $\log[\mathrm{Fe}^{++}/\mathrm{Mn}^{++}] \sim -0.45 + 0.57 \sim 0.1$. This should be compared with our estimate of +0.57, from the plots, taken without a painstaking regard of the actual distributions of intensities and wavelengths of the two line sets. The difference, 0.5 dex, or a factor of 3, is probably representative of the uncertainties of the present method.

TABLE 6

INTERCOMPARISON OF WCS FOR 100 MATCHED Mn III AND Fe III LINES

	Max	Min	Mean	S
λ(Mn III)	1998	1512	1908	5.45
log [IP(Mn III)]	−2.72	−5.18	−4.51	
λ(Fe III)	1999	1506	1849	3.63
log [IP(Fe III)]	−2.69	−5.27	−4.50	
λ(Mn III)	2433	1982	2107	2.73
log [IP(Mn III)]	−2.55	−4.41	−3.89	
λ(Fe III)	2339	1980	2058	3.25
log [IP(Fe III)]	−2.55	−5.17	−3.25	

The results with the matched wavelengths in the LWR region give lower significance parameters, but indicate that the Fe III lines are somewhat stronger than the Mn III. The difference, 0.52, in the S-parameters corresponds to 0.09–0.17 in $\langle \log(\mathrm{IP}) \rangle$. The mean, 0.13, would give, by equation (4), a value of $\log(\mathrm{Fe}^{++}/\mathrm{Mn}^{++})$ of 0.7, which seems high, but is not out of line with some of the values listed in Table 1, or our earlier result of +0.57 obtained from plots similar to those of Figure 1.

Our findings may now be succinctly stated. We find no evidence of departures from Saha equilibrium in either the iron or manganese ionizations (single to doubly ionized stages). If there are effects due to the concentration of Mn to a high, presumably cool layer, they change the level of ionization from that expected by no more than a factor of about 3. We cannot exclude the possibility that large departures from Saha equilibrium are canceled by the effects of layering.

The iron and manganese abundances are within a factor of 3 of one another. These findings are subject to an overall uncertainty of 0.3–0.5 dex, and departures from ionization equilibrium *within these limits* can by no means be ruled out. However, our results are in good agreement with the large excesses of manganese found in earlier abundance work on κ Cnc.

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