

*Section V. Spectroscopy and astrophysics***ON THE COMPLETENESS OF THE ANALYSIS OF THIRD AND FOURTH SPECTRA OF THE IRON GROUP, AND THE SPECTRA OF EARLY B STARS**

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The spectroscopic analysis of normal, early B stars requires a sound atomic data base, especially for the third and fourth spectra of the iron-group elements. We review the present status of the term analyses of third and fourth spectra of vanadium–nickel as of the Sugar–Corliss compilation. Incompleteness of the analyses of the third spectra is typically evident about halfway to the first ionization limit. The fourth spectra are less well known. For Fe, Co, and Ni IV, only the lowest three configurations have been located.

Copernicus spectra described by Rogerson and his coworkers have been studied in detail. We conclude that present atomic data is approaching a sufficient degree of completeness to allow a realistic analysis of the satellite ultraviolet of the “normal” star. Without analytical work of the last decade, the analysis of the UV spectrum of this star would have been hopeless.

1. Introduction

The satellite ultraviolet spectra of early B stars are replete with lines that come primarily from iron group elements. Rogerson and Ewell [1] (henceforth RE) measured 3576 wavelengths in the Copernicus spectrum ref. [2] of τ Sco, possibly the most thoroughly studied of these stars. In their detailed examination, RE suggested identifications for 61% of the measured wavelengths ($\lambda\lambda 948$ – 1560). We summarize some of their results in table 1, which lists the number of wavelengths identified with spectra from the iron group. It is convenient to list in the same table, partition functions calculated for 31 000 K, which give some indication of the richness of an atomic spectrum; the temperature is near that for the photosphere of the star τ Sco.

This table is interesting from a number of viewpoints. Note that the spectra listed include some 83% of all of the 2194 identified lines, and more lines of Fe III were identified than of any other species. This is to be expected from the richness of the spectra of these transition elements, and the relatively high cosmic abundance of iron. Solar abundances are shown in fig. 1 (cf. ref. [3]).

The absence of V III and the small number of identifications in Ti III–V IV are not discussed here. They may be due to the relatively low abundances of titanium and vanadium in τ Sco, as well as the relatively small number of predicted lines from these spectra.

Cowley and Merritt [4] recently completed a study of International Ultraviolet Explorer (IUE) spectra of τ Sco, in addition to the published Copernicus data. They noticed that RE had identified more Mn III lines in τ Sco than Cr III, and noted this was surprising because they were able to establish the presence of Mn III only with considerable difficulty, by the technique of wavelength coincidence statistics (WCS). This may be because there were more known laboratory Mn III than Cr wavelengths. Chromium is slightly more abundant cosmically than manganese, and the partition function for Cr III is larger than for Mn III. We would therefore expect, *cet. par.*, more Cr III lines *in the star*. Is this actually the case? Are there really more Cr III lines in the stellar spectrum than it was possible to identify because of missing data?

A satisfactory answer to this question cannot be given at this time. We anticipate that Dr. R.L. Kurucz will complete calculations of oscillator strengths in Cr

Table 1
Number of identified lines of iron-group spectra partition functions for 31000 K (total number of lines: 1817.)

Spectra	No.	Parfn.	Spectra	No.	Parfn.	Spectra	No.	Parfn
Ti III	16	39.8	Cr IV	257	61.1	Co III	18	71.2
Ti IV	7	10.0	Mn III	304	51.6	Co IV		62.8
V III		79.7	Mn IV	19	61.0	Ni III	54	39.6
V IV	8	32.7	Fe III	626	89.2	Ni IV	73	52.6
Cr III	276	96.7	Fe IV	159	32.2			

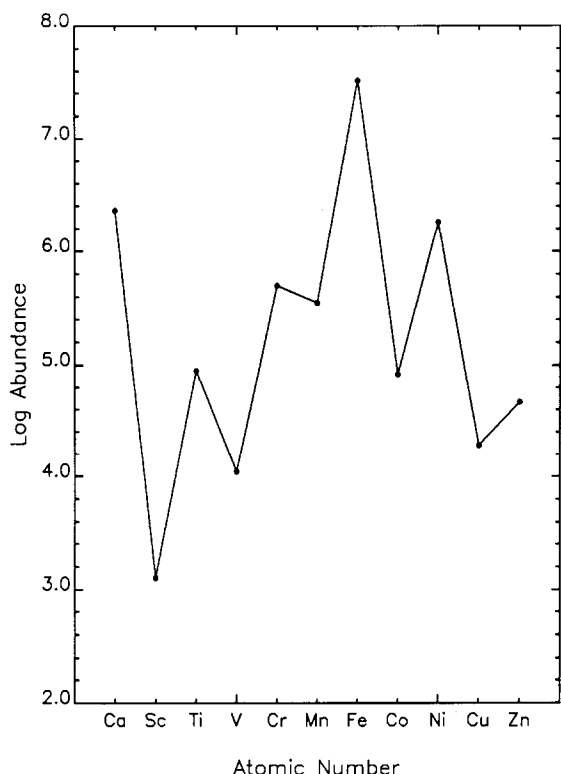


Fig. 1. Solar abundances of iron-group elements. The normalization is chosen so that the hydrogen abundance is 10^{12} . Note that the abundance of iron is some two orders of magnitude higher than the abundances of chromium, manganese, or cobalt.

III and Mn III that will enable us to answer this question (cf. [5]).

The absence of any identifications in Co IV is worth attention. Only the lowest three configurations of this ion are known, and many of the wavelengths given by Kelly [6] are only to the nearest 0.1 \AA . Lines in the transition array d^6-d^6p fall short of the stellar wavelength coverage, while those in $4s-4p$ are at the extreme, long-wavelength end of the Copernicus data. We have examined a few of the relevant regions with IUE material, which extends to ca. $\lambda 3200$. We did not reach a firm conclusion on the presence or absence of Co IV. A statistical study of the ion using WCS would have been appropriate. Unfortunately, without accurate wavelengths, an analysis by WCS is of questionable value.

Again, we are in need of the kind of calculations provided by Dr. Kurucz. While the term analysis of Co IV, like that of all fourth spectra of the iron group, needs to be extended, useful information could be obtained from existing energy levels, which have been updated since the Kurucz-Peytremann [7], henceforth, (KP) study.

In this paper we discuss a survey of third and fourth spectra of iron-group elements relevant to the general question of whether our knowledge is sufficiently complete to allow a thorough analysis of the spectra of early B stars such as τ Sco.

2. Completeness of the analyses: third spectra

The material for this section is based on a digitized version of the recent compilation by Sugar and Corliss [8]. It is a straightforward, though tedious programming project to search each spectrum for identified configurations, and in addition, to count the number of elementary states that belong to the classified levels of each configuration. These counts are compared with the theoretical expression

$$\sum g_i = \prod_{i=1}^n \binom{4l_i + 2}{w_i}$$

for the number of states from configurations of the form l^n (cf. Cowan [9] eqs. 4.65 and 21.9).

The results for the survey are shown for the third spectra in tables 2a and b. Logically, Ti III and IV might have been included. Our focus has been on what the nuclear astrophysicist calls the "iron peak" rather than the spectroscopist's iron group. Beside each configuration, we give the following information: the ratio L/Ion of the lowest level belonging to the indicated configuration to ionization, the weight of the configuration according to the relation above, and the ratio Kn/Pre of the weights of known levels to the predicted weights. The order of the configurations in V III is followed for all 6 ions.

It is immediately apparent that configurations with their lowest levels ca. halfway to ionization are only partially analyzed. No levels are known above the ionization energies in any of these spectra.

Fortunately for the astronomers (see fig. 1) Fe III is the most thoroughly analyzed of these spectra. Cr III and Co III need the most work.

Johansson [10] noted that the relatively low-lying configurations $3d^k-2s^2$ were absent from analyses of most third spectra of the iron group. Corresponding configurations are known in the first and second spectra of vanadium through nickel, and include the ground term of Mn I–Ni I. Among the third spectra, $3d^k-2s^2$ is known only in Ni III, where two levels from the ground term 5D are located at 153.2 and 154.17 (10^3 cm^{-1}). According to Kurucz [11] these levels are mixed with $3d^7(^4F)4d$, which accounts for a variety of transitions to upper levels belonging to $3d^7(^4F)4f$ with moderate values ($-2.0 < \log(gf) < -1.0$) of the transition probabilities.

These $3d^64s^2-3d^74f$ transitions in Ni III have not been established in τ Sco. Analogous transitions in Fe

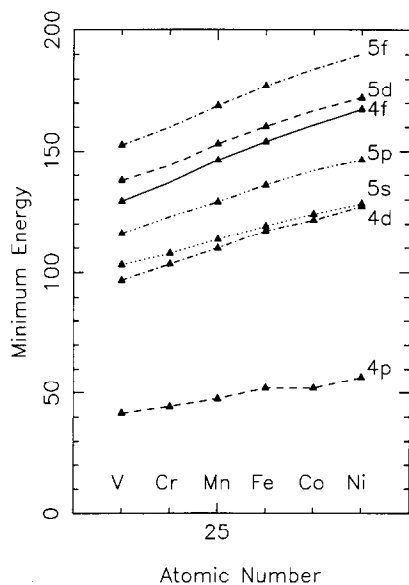


Fig. 2. Energies (in 10^3 cm^{-1}) of the lowest levels of some configurations of third spectra of iron-group elements relative to the $3d^{k-1}4s$. The symbols represent known configurations; positions for unknown configurations are interpolated. Points for the $3d^{k-1}6s$ are not shown. They would fall very near those for $3d^{k-1}5d$, and interpolations are required for Cr III and Co III.

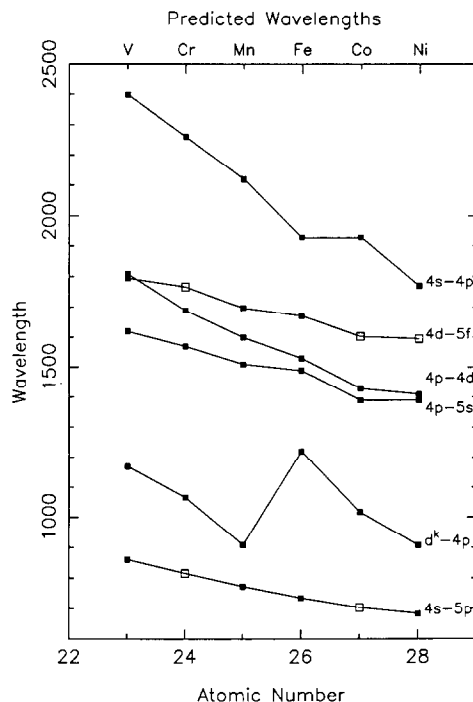


Fig. 3. Predicted wavelengths in ångströms of transition arrays from using the data of fig. 2. The open symbols show transition arrays involving a predicted configuration.

locations of missing configurations, and transition arrays. The configurations $3d^35p$, $3d^34f$, $3d^35d$, $3d^36s$, and $3d^35f$ in Cr III and analogous configurations ($3d^3nl$) in Co III may all be located approximately by these methods. In Mn III, the lowest levels in the corresponding configurations ($3d^45p$, etc.) are known. Some curves of this kind are shown in fig. 2. With the help of such curves, we can predict "a" wavelength that is relevant to the transition arrays, for example, in Cr III: near $\lambda 850$ ($4s-5p$), $\lambda 2980$ ($4d-4f$), and 1750 ($4d-5f$) (see fig. 3).

The rich $4s-5p$ transition array in Cr III will have its strongest lines short of the Lyman limit ($\lambda 912$), a domain that is inaccessible in most stars because of absorption by interstellar hydrogen. However, since the totality of the transitions in arrays such as these spread over a considerable wavelength domain (see fig. 4 below), $4s-5p$ transitions should be detectable in satellite spectra, especially of stars with enhanced chromium abundances.

We illustrate some of these transition arrays with the help of the relatively well known Fe III spectrum. Kurucz [5] has kindly made available new calculations in this spectrum. With the help of his oscillator strengths and the level classifications tabulated by Sugar and Corliss, it is straightforward to identify lines belonging to a given transition array. We plot an intensity parameter,

calculated for the τ Sco atmosphere (cf. ref. [4]) vs wavelength. The intensity parameter is essentially the logarithm of the gf-value times a Boltzmann factor. An abundance and ionization factor is included, but this is an additive constant for all of the lines of Fe III.

Fig. 4 shows the rich $4s-4p$ array, while fig. 5 shows several other arrays. The arrows indicate the wavelengths from fig. 3. The strongest lines in the transition

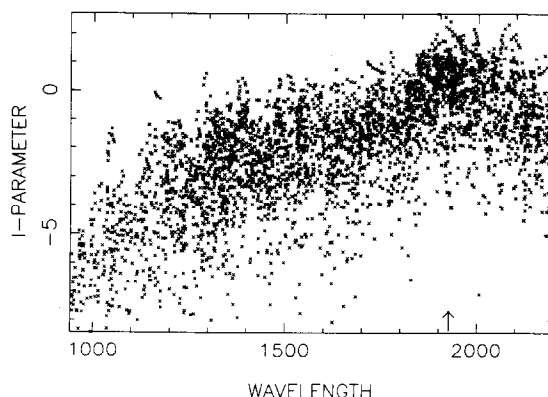


Fig. 4. Logarithmic intensities vs. wavelengths for Fe III lines in the rich transition array $4s-4p$. The arrow shows the wavelength predicted from fig. 2.

well known than the third spectra. For Fe, Co, and Ni, only the lowest three configurations are known. Is this important from the viewpoint of the stellar spectroscopist?

Let us consider the case of Fe IV. The study by Ekberg and Edlen [13] is essential to any astronomer who wishes to understand the ultraviolet spectra of early B stars. Moore's An Ultraviolet Multiplet Table [14] does not even include Fe IV, while the KP tables were based on a provisional study by Edlen [15]. Kelly and Palumbo [16] list only 19 lines of Fe IV with $\lambda < 700 \text{ \AA}$.

The Ekberg and Edlen work is included in the compilation by Kelly in Wiese's valuable Spectroscopic Data for Iron [17], but this list is surely not extensive enough to allow a complete analysis of the τ Sco spectrum. For example, none of the 20 lines for which KP calculated transition probabilities, are included. These KP lines are all intersystem transitions, but several were identified by RE with moderately weak stellar absorption. Such identifications are characteristically very subjective, but we judge them to be essentially correct.

In order to get an unbiased indication of the presence of weak Fe IV features, we performed a WCS test on the weakest 108 lines in the Kelly list. These lines were primarily at wavelengths longer than the Copernicus data, so the search was made from measurements of the noisier IUE material. We confirmed that these weak lines were indeed present at a very high confidence level ($> 99.5\%$).

Additional levels in Fe IV are therefore needed. Transitions involving 4d, 5s, and 3d²4s4p could very probably be found in τ Sco if they were known. A star with an enhanced iron abundance whose temperature was the same as that of τ Sco would be expected to have many lines due to Fe IV that could not be identified with present material.

4. Rediscussion of identification in τ Sco: a sample region

The study of τ Sco by Rogerson and Ewell (RE) was of very high quality. The most up-to-date compilations of atomic data were employed, and calculations were made to predict the expected strengths of features in those instances where oscillator strengths were available. The major results of their work were presented in the form of two tables giving identifications for some 61% of the 2194 measured wavelengths. Cowley and Merritt [4] analyzed the Copernicus material as well as IUE spectra using the method of wavelength coincidence statistics (WCS). They suggested that the 61% identification rate might give an overly optimistic assessment of the percentage of correctly assigned absorption.

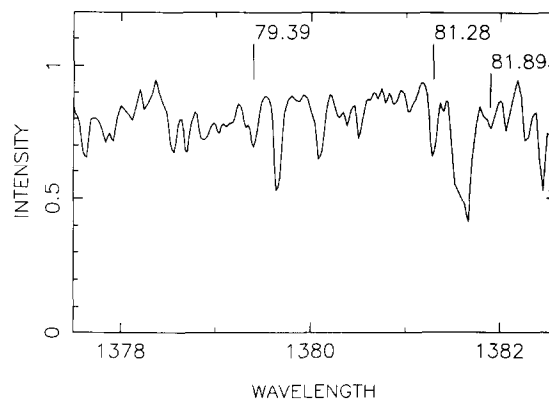


Fig. 6. Sample region of the Copernicus spectrum of τ Sco. The strongest features are intensity 5, the weakest, intensity 0. The S/N ratio is about 35, so that the individual intensity-0 features are severely perturbed by noise. Plausible identifications can be given for the majority of the stellar wavelengths.

An independent check on the identifications of (primarily faint) features in τ Sco can be made in the least two ways. One method is to perform WCS tests using species expected to be faintly present. Such tests are discussed by Cowley and Merritt. A second method is to make use of new material, unavailable to earlier workers, Kurucz [5] has kindly made such new material available in the form of a data tape containing semi-empirical oscillator strengths for iron-group spectra. For our purposes, the most important spectra for which the new calculations were available were those for Fe III, Co III, and Ni III.

We selected a 25 \AA test region of the τ Sco spectrum, and made a feature-by-feature examination. We discuss here, a subset of stellar wavelengths $\lambda\lambda 1375.050$ – 1382.451 . The 56 wavelengths in this region were assigned intensities on a scale of 0 (roughly 1 to 2 m \AA) to 5 (some 100 m \AA). The distribution of lines with various intensities is as follows: intensity 0, 22 lines; 1, 16 lines; 2, 13 lines; 4, 2 lines; 5, one line. Fig. 6 shows a portion of the stellar spectrum.

The intensity-5 feature at $\lambda 1381.647$ cannot be considered satisfactorily identified. RE marked it with an "a", whose meaning we summarize with the word "problematical". It is partially due to P III and C III. The principal contributors to the two intensity-4 lines are credibly assigned by RE. One of the intensity-3 lines, $\lambda 1380.289$, was unidentified by RE. We can find no plausible suggestion for it. The other, $\lambda 1380.096$ was marked with an "a", and partially attributed to $\lambda 1380.112$ of Fe V. Ni III $\lambda 1380.05$ must contribute to the feature as well.

Of the 13 intensity-2 lines, 3 were unidentified by RE. We find Ni III $\lambda 1382.09$ is a plausible identification for one of them. Co III $\lambda 1378.67$ may contribute

to one of these lines, while the other, $\lambda 1379.402$, remains unidentified. For 4 of the intensity-2 features marked with an "a" by RE, we could find no additional contributors.

Among the 17 intensity-1 lines, $\lambda 1381.900$ remains unidentified. We could suggest plausible assignments or additions to 7 features, while 8 remain as assigned by RE.

RE left 10 of the 20 intensity 0 features unidentified. We could suggest plausible contributions for about half of them. The reality of the weak features in this wavelength domain is questionable. The signal-to-noise ratio is only about 35.

The notion of whether or not a stellar absorption feature is "identified" is hardly a crisp one. The ideal approach is that taken by Kurucz and his coworkers (cf. ref. [18]), who make a direct comparison of the observed and theoretically computed spectrum. Lacking such calculations, we offer the following conspectus. Some of the lines within our test region, we judge to be identified without any doubt. If all of our questionable assignments are correct, 51 out of 56 lines (91%) are identified. If they are all incorrect, 26 of 56 (46%) are identified. If reality lies halfway between these extremes, the relevant percentage is about 70. This is an improvement over RE's result, and is encouraging.

From a less intensive study of the region $\lambda\lambda 1375-1400$, it appears that the results presented above are representative of the wider, 25 Å region, and we assume here they are typical of the ultraviolet spectrum of τ Sco. We summarize as follows:

- 1) The majority of the strong features (intensity 2 and stronger) were correctly assigned by RE.
- 2) For about half of the weaker features, there are significant additional contributions to those suggested by RE.
- 3) The new data from Kurucz [5], on Fe III and Ni III alone, has made a significant contribution to the identifications in τ Sco. Additional material for the third and fourth spectra may make it possible for a realistic analysis of weak features in the spectra of normal stars of this temperature.
- 4) For the present, the analysis of the weaker features in τ Sco is still plagued by questions of incompleteness of atomic data.

5. Conclusions

Additional work needs to be done on the spectra of iron-group elements before they can be considered satisfactorily analyzed from the viewpoint of the stellar spectroscopist. Nevertheless, it does seem that the basic data is close to being sufficient for a reliable analysis of the ultraviolet of a fairly normal star such as τ Sco.

This conclusion lends strong support to the approach taken by Kurucz, who has attempted to provide global atomic data on literally millions of spectral lines. We hope this will act as an incentive to the laboratory spectroscopist to continue the difficult but essential work of term analysis of complex atoms.

We clearly require additional calculations of the kind provided by Kurucz. Extended analyses of the fourth spectra of all of the iron group would be welcome in order to provide the basis for additional semi-empirical calculations.

In the present discussion, the demands on our knowledge of the spectra of elements other than iron have not been severe because of our choice of τ Sco, a star with arguably "solar" abundances (cf. fig. 1). It is well known that some slightly cooler stars have greatly enhanced abundances of iron-group elements. In some peculiar stars, iron may be enhanced with respect to hydrogen by more than an order of magnitude, while chromium and manganese are often enhanced by two orders of magnitudes.

We do not yet know if any of the early B stars have such enhancements of iron-group elements. Spectra obtained from the ground show essentially only the abundant light elements, such as helium, oxygen, nitrogen, neon, etc. It is palpably plain that the early B analogue of α^2 CVn would have a UV spectrum replete in lines of Cr III and IV for which identifications are not yet possible.

For the present, the abundance worker is well advised to work with strong lines, on the damping portion of the curve of growth. The more interesting, and in principal more accurate information available from weak features, is still not yet available because of a dearth of basic atomic data.

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