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J.G. Phillips and G. Traving

ATOMIC ENERGY LEVELS AND SPECTRA: ASTRONOMICAL NEEDS

Charles R. Cowley
University of Michigan
Dominion Astrophysical Observatory

I. Introduction

The astronomer's requirements for atomic data are so massive that it is not easy to approach this subject in a way that will sound responsible to someone who is not thoroughly familiar with the situation. The simple truth is that there is hardly an atomic species, neutral or ionized, for which additional data is not urgently needed in some domain of astronomy. This comes about partly because of the high temperatures and very long path lengths in astronomical objects which can make them extremely powerful light sources. More generally, we can say that conditions in the astronomer's violent universe manage to render large volumes of phase space available to the atoms which occupy it.

While the truth is that we need to know "everything," one task of the present paper is to cast this need in a pragmatic form. This will be done by reviewing certain problems in the very recent history of astronomical spectroscopy, where real progress has come about as a result of new work on atomic spectra. Many of the illustrative problems are taken from the spectroscopy of upper main sequence, chemically peculiar or CP stars.

We apologize for a total omission of the very active field of atomic and solar spectroscopy dealing with highly ionized species. Fortunately, Cowan's (1981) new book includes a chapter on this topic, along with many references.

It is inevitable that many of our requirements are for tedious, routine analyses of atomic systems, for which a principal motivation is the astronomical application. Let us therefore state briefly why work in this domain is so interesting.

The fascination stems from the appeal of the unknown. The CP stars have a rich, variegated surface chemistry for which our present understanding is at best rudimentary. We know the chemistry is unusual because of the spectra, but quantitative abundance determinations are fraught with many uncertainties, partly stemming from physical and partly from astrophysical shortcomings.

Moreover, we do not have a clear idea of why the peculiar chemistry occurs. It may be that we stand on the threshold of an entirely new discipline of "stellar geochemistry" in which clues to the internal fluid dynamical and nuclear history are read from the surface composition. Alternate ideas about these stars would call upon entirely new modes of stellar evolution and nucleosynthesis. There is an empirical connection between certain chemical peculiarities and stellar magnetism that represents an entirely open domain for future work.

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Real progress in understanding these stars promises rich rewards.

Because astronomy is an observational science, many observations are analyzed by the technique of modeling. This means all relevant physics must be put into the model if it is to have any hope of success - success comes when the model fits the observations.

Older work in solar and stellar spectroscopy used a "partial" modeling technique based on measurements of individual spectral features that were (thought to be) dominated by an identifiable atomic species. Such a procedure is still useful in many situations, but it cannot deal realistically with the severe blending that is found in the satellite ultra-violet of normal stars or even of ground-based spectra of some CP stars. Here we must have recourse to the numerical synthesis of the stellar spectrum.

Two approaches have been taken by astronomers who do this work. Bell, Gustafsson, and their coworkers (cf. Bell and Gustafsson 1978) have used observed atomic lines, taking as their basic source the tables of Moore, Minnaert and Houtgast (1966). Their method has had considerable success in dealing with ground-based spectra of late-type stars. It has not been extensively applied to CP stars, or their "normal" upper-main sequence congeners, and lack of atomic data precludes its usefulness much below, say, λ2700.

Kurucz and Peytremann (1975, henceforth KP) provided the basis for spectrum synthesis using an atomic line list generated by theoretical atomic structure calculations. Their tables contain some observed lines, but the bulk of the work is based on lines generated from atomic energy levels. This work was a fantastic achievement. Certainly, one may improve upon its detailed results (cf. Kurucz 1981), but it is difficult to see how the work might be improved in concept or scope.

One severe limitation, which certainly affects the overall success of KP's method is the lack of knowledge of energy levels. Even when transitions involving unknown levels do not produce important lines, the levels may be mixed with others in such a way that important transition probabilities cannot be calculated accurately. At the present time, such mixing is regarded as one of the primary causes of inaccuracy in theoretical calculations of a global nature such as those of KP.

Let us consider some illustrative examples. The first will come from the sun rather than the CP stars. Figure 1 is from Kurucz and Avrett's (1981) attempt to synthesize parts of the solar ultra violet. The atomic data is from KP. One can see from Figure 1 (bottom) that between λ2897 and 2899 the calculations bear some resemblance to the observations. From λλ2289 to 2291 the exigent need for more opacity sources in the theoretical calculations is apparent.

Table 1

Tabulated Atomic Lines λλ1361-1363.5

Source	No. lines I-III
UV Multiplet Tables (1962)	6
Kelly and Palumbo (1973)	28
Kurucz and Peytremann (1975)	89
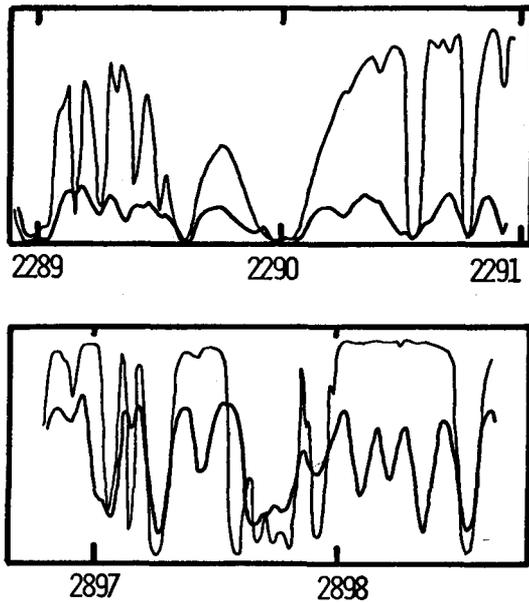
Figure 1: Observed (thick line) and synthesized (Kurucz and Avrett, thin line) solar spectrum in two ultraviolet wavelength regions. The calculated spectra fail to match the observed features because of opacity sources that are for the most part unknown.
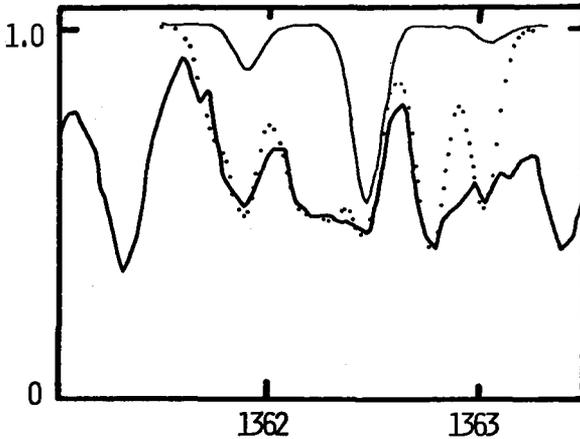
Figure 2: Vacuum ultraviolet tracing of ν Cap (thick line) in the region of the strong B II line λ1362.46. The solid line was synthesized by Leckrone using lines and transition probabilities directly from KP. Dotted spectrum computed with modified log (gf)'s.

A second example is taken from the work of Leckrone (1981). Figure 2 shows the UV spectrum of ν Cap, a "normal" B9.5 V, in the region of the strong B II line λ1362. The observed spectrum is shown as a thick, solid line. Two theoretical (calculated) spectra are shown. The thin line gives calculations based on lines and gf-values directly from KP, combined with solar abundances believed to apply to ν Cap. The dotted line incorporates empirical adjustments to KP required for a best fit to the observed spectrum. Some of these adjustments are considerable, as we shall see. The serious incompleteness of laboratory data in this critical region is well illustrated in Table 1 which gives wavelengths in the region λλ1361-1363.5. The first two sources are of observed lines, while the second includes predicted lines.

Table 2 lists three sets of oscillator strengths for six Fe II lines within this region. The first set is from KP. The second is from Kurucz's (1981) substantially improved calculations, while the third set represents the empirically adjusted log (gf)'s necessary for the optimum fit shown in Figure 2. The last column, Δ, is the difference of the previous two. A negative value of Δ means more opacity is required than can be accounted for at present.

Leckrone's empirical adjustments are surely a constructive step, but strong opacity sources are still missing. For an arbitrary feature, it is virtually impossible to know whether the oscillator strength in KP is too small, or if additional "unknown" lines are responsible for the extra opacity.

Table 2

Fe II Log(gf) Values

λ	KP	K-81	Empirical	Δ
1361.86	−4.69	−3.96	−2.40	−1.56
61.93	−3.61	−3.08	−2.70	−0.38
62.07	−7.05	−2.55	−2.10	−0.45
62.69	−6.93	−5.77	−6.93	+1.16
62.77	none	−0.81	+0.30	−1.11
63.02	−8.94	−9.61	−1.60	−8.01

The ground-based photographic spectra of certain CP stars can be just as much of a jumble as the satellite UV of the sun and "normal" stars. The following illustrations are from Cowley et al. (1977). Figure 3a shows an intensity tracing of the region of the so-called unblended U II line λ3854.7. In fact, both of these features are dominated by Cr I in this and many other Cr-rich Ap stars. The Cr I lines near λ3859.6 have not been observed in the laboratory, but they do appear in KP's tables (Cowley and Arnold 1978).

Now the critical fact is that λ3859.6 is dominated by U II in a few CP stars where Cr I is weak. Before looking at our example, note the strength of Cr I λ3858.9 in 73 Dra. Consider the nearest feature to this Cr I line in Fig. 3b which is from the rare-earth maximum spectrum of HR 465 (see below). There is a strong feature nearly two tenths of an angstrom away which must be primarily some other species.

We have not been able to identify the principal contributor to λ*3858.73 but its position is incompatible with an identification as Cr I. Consequently, we may be sure that Cr I is weak in this stellar spectrum, while λ3859.6 is still quite strong, undoubtedly because of the contribution from U II. It is just this phase in
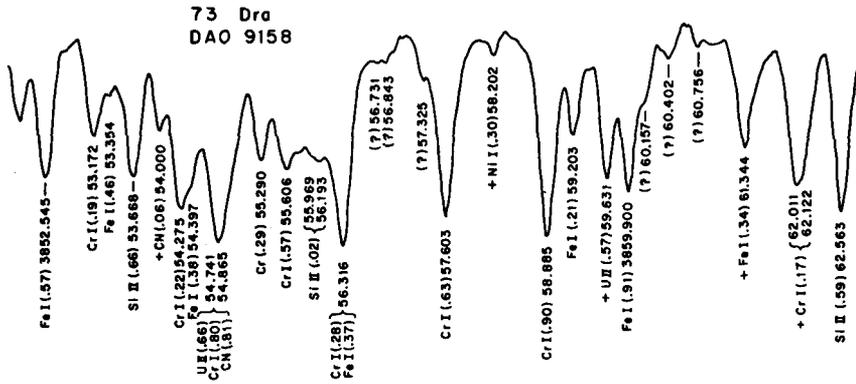
Figure 3a: Intensity tracing of 73 Dra in the region of two U II lines. Identifications of measured stellar wavelengths are given. Decimal fractions of laboratory wavelengths are given in parenthesis.
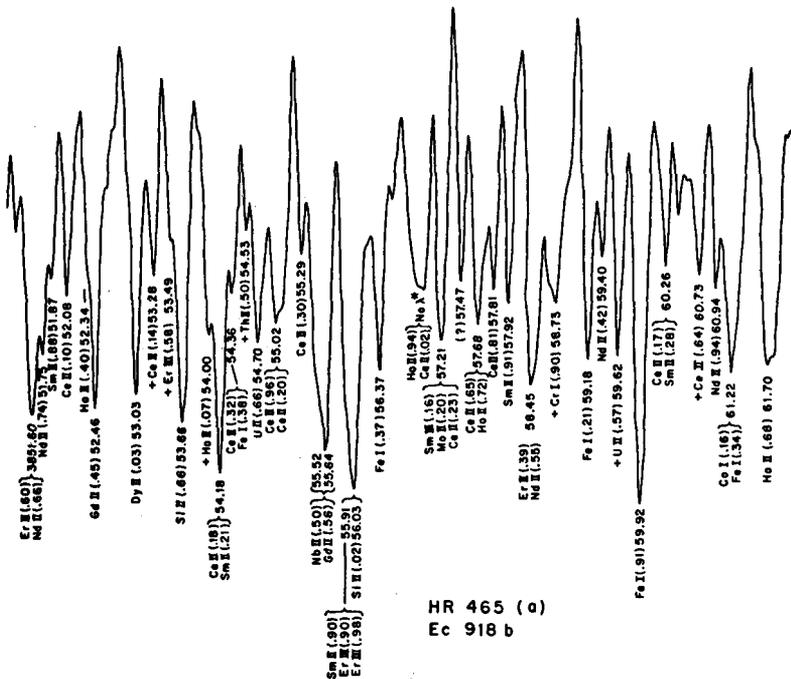
Figure 3b: Intensity tracing of the rare-earth maximum spectrum of HR 465.
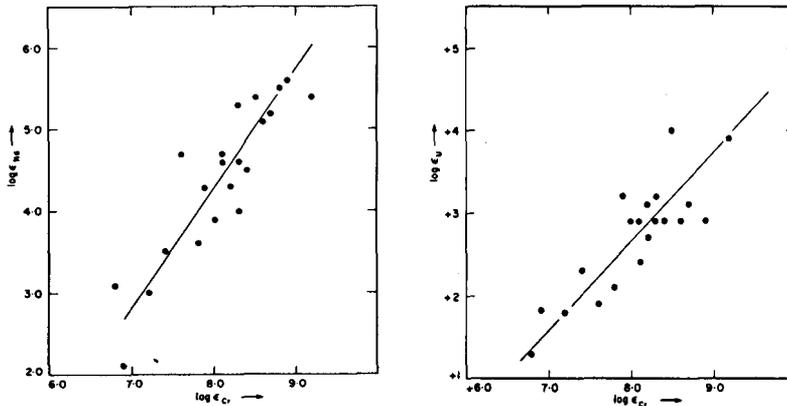
Figure 4ab: Spurious, induced correlations of abundances of exotic
elements in CP stars resulting from unrecognized elements in CP stars
resulting from unrecognized blends with Cr I and II. Noedymium (left)
and Uranium (right) abundances are plotted vs those found for
chromium. (Courtesy of the University of Chicago Press).

the spectrum that wavelength coincidence statistics (WCS) support the identification
of both uranium and thorium, the latter from second as well as third spectra (see
Cowley and Rice 1981). Note the richness of the rare-earth lines as well as
contributions from the third spectra. The Er III wavelengths are from unpublished
material kindly made available by Hannah Crosswhite.

There is a moderately strong absorption feature in many CP stars near the
strongest Nd II line of Meggers, Corliss, and Scribner (1975), $\lambda 4303.58$. Stellar
spectroscopists have used it to obtain neodymium abundances. In fact, the feature
is primarily due to a predicted Cr II line in most CP stars, and this gives rise to
a remarkable and purely spurious correlation between chromium and neodymium
abundances in magnetic CP stars (Cowley 1981), illustrated in Figure 4a. A similar
spurious correlation with uranium abundances is expected on the basis of the above
discussion of blends of Cr I with U II lines. It can be seen in Figure 4b.

The moral of these stories is that we cannot understand what is going on with
exotic and trace species without complete information on what may otherwise be
uninteresting transitions in common ions. The particular cases illustrated in this
subsection are ones in which KP has so to speak, come to the rescue, but many
puzzles remain.

One more illustration from our zoo of CP spectra is shown in Figure 5 from
Aikman et al. (1979). The top spectrum, of γ Equ, is moderately rich in lanthanide
rare-earth lines. The lower spectrum is of HR 465, which is somewhat hotter. A
strong Dy III line is indicated. Note also the Nd III line at $\lambda 3920.18$, partially
blended with Fe I $\lambda 3920.26$. The measured wavelengths indicate the stellar features
are dominated by Fe I in γ Equ and by Nd III in HR 465. Both of these features were
identified with the help of unpublished material kindly made available by H. M. and
Hannah Crosswhite.

Aikman et al. made a provisional list of Dy III lines from Hussain's (1973)
melange from various dysprosium ions, eliminating Dy I and II with the help of
Conway and Worden's (1970) huge list, and assuming that Hussain's Dy IV would not
appear in stellar spectra. Sugar and Specter (1974) have photographed the Dy III
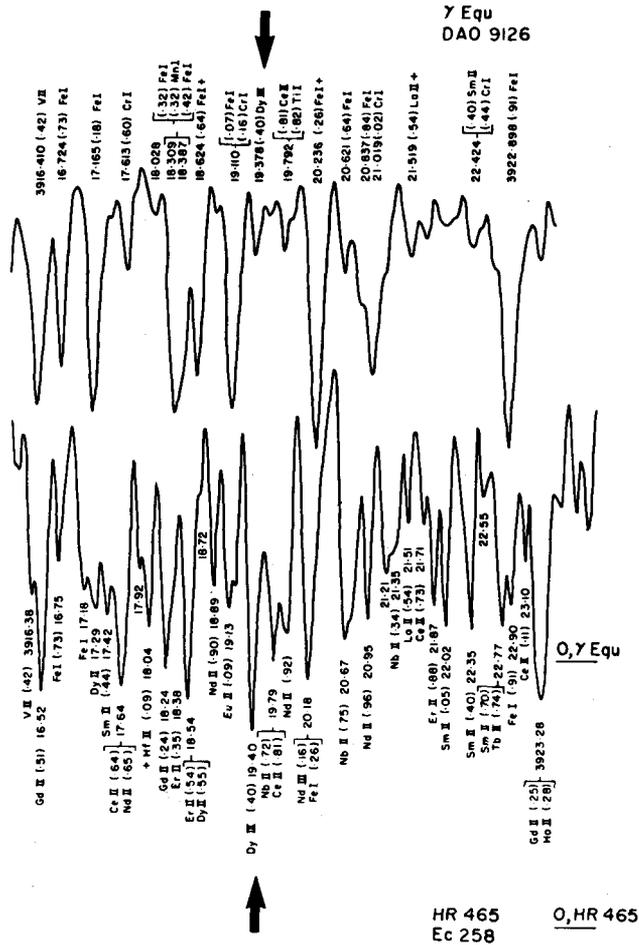
Figure 5: Intensity tracing near a strong Dy III line in two CP stars. Zero intensity for γ Equ and HR 465 are indicated on the right. (Courtesy of the University of Chicago Press).

spectrum, and only about one third of our lines are in their list (Sugar 1978). It thus remains entirely possible that some of our "provisional Dy III" lines are from high level lines in Dy II.

This is only one of many possible illustrations where we need more information about the lanthanides in order to understand what is going on in the spectra of CP stars.

II. Atomic Spectra: General Remarks

Let us now turn to a consideration of atomic spectra per se. We cannot review the entire domain. Cowan (1981) provides a very useful table which "grades" the analyses of up to 51 stages of ionization of 100 elements. From the point of view

of astronomers, further work is badly needed even in spectra with the highest grades of analysis assigned by Cowan, and we shall illustrate this specifically with a consideration of iron group.

The best way to survey an atomic spectrum for completeness would be to make ab initio calculations of all possible levels, and compare them with the compilations. Existing programs might easily do this but this writer does not presently have results from such comparisons. We must content ourselves with some general considerations and a few specific probes.

Obviously, atomic analyses will never be complete in the ideal sense. At any given time, or let us say with any particular issue of the J. Phys. Chem. Ref. Data, the levels will be known up to some maximum term value, which we shall call T_S. (The phrase "term value" as used here means the energy in cm^{-1} measured from the ground state.) This may or may not be higher than T_I, the ionization energy in cm^{-1}. Sometimes the incompleteness of an analysis is apparent, as when T_S is only about half as large as T_I. The blatant incompleteness of known levels in many lanthanide spectra reveal themselves in this way. In better-studied ions, we need only slightly more sophisticated methods to discover the incompleteness.

In the second and third spectra or iron-group elements, we have tried to locate an approximate (NB) value T_H where expected terms are no longer regularly found. In cases where some special series have been experimentally pursued, T_H can be markedly lower than T_S. We shall call T_H the top of the heap, and T_S the top of the stack. Our placement of T_H is very rough, and a more thorough exploration of these spectra may put it lower.

We attempted to gain some insight into the location of T_H from histograms of tabulated energy levels, but this is not easy to do. Figure 6a shows the Fe II spectrum before (Reader and Sugar 1975), and after the work of Johansson (1978). Although many levels were added by Johansson above 87.5 kK, we find evidence (see Table 3 below) that the top of the heap for this spectrum is in the region 90-95 kK.

In Cr I, a number of levels are known above the ionization limit (see Figure 7b), but a simple check reveals the top of the heap of "complete" levels is well below the ionization limit of 54.5 kK, indicated by the arrow (Sugar and Corliss 1977).

The technique used in this paper to probe for missing levels has been rather simple. Energy spacings for parent terms were found from the tabulations for the "next higher" ion. Then allowed groups of terms with the configuration $d^k(LS)nl$ were sought with fixed nl, for successively higher allowed parent terms. The intervals between the centers of gravity of resulting terms with the same multiplicity are roughly those of the parent ion. In this way, for example, we find that terms built on $d^5(LS)4s$ can be followed in Cr I to less than 40 kK, which is well below the top of the stack (highest known level) for the atom.

The Cr I spectrum is of special interest to students of CP stars as a result of situations such as those described above for the U II blends. We can be sure that since the predicted Cr I (and Cr II) lines are strong in our stars, a knowledge of new levels will allow identifications of still more lines. Confirmation of this should be available through work by Johansson (1982) to be reported at these proceedings.

Figure 7 shows the distribution of the known Cr II levels from Sugar and Corliss (1977). The ionization energy is 133.0 kK, and one can perhaps sense the incompleteness of the analysis from this plot alone.

Both R. A. Bell and R. L. Kurucz note incompleteness in line lists and energy levels of Fe I. This spectrum, of course, illustrates one of the classical cases
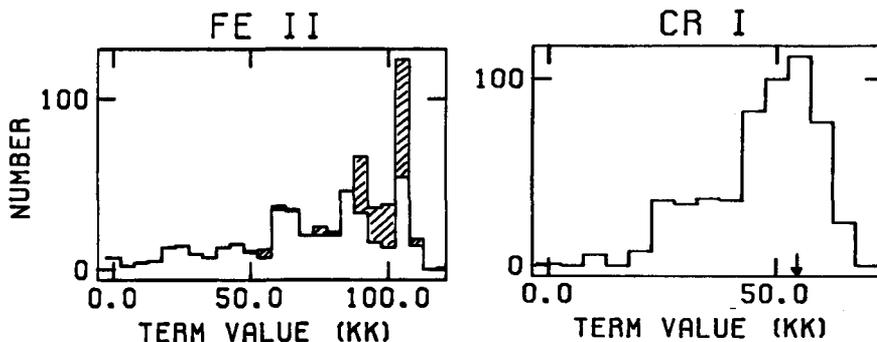
Figure 6ab: Histogram of energy levels for Fe II (left) and Cr I (right). Johansson's work in 1978, indicated by the shaded areas, greatly increased the number of high levels in Fe II.
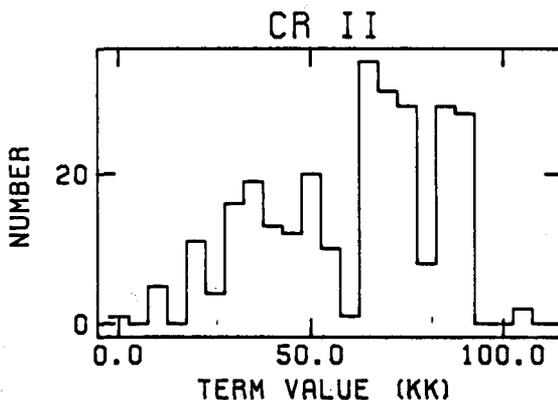
Figure 7: Histogram of tabulated Cr II levels in 1977. Ionization is at 133.0 kK.

where predicted lines were identified in an astronomical source. However, Fe I is considerably stronger in late-type giant stars than in the sun, where the predicted Fe I lines were first identified. These late giants are currently of great interest because of recent work on abundances in distant stellar systems such as globular clusters and galaxies.

Jamar (1980) called attention to the astrophysical importance of autoionizing levels in Fe I on the photoionization cross section. The experimental work reported by Hansen et al. (1977) only treated transitions from the ground level. Naturally we must know the cross section from other levels for accurate calculations.

Another common atomic spectrum that badly needs modern work is Ti I. Some low terms are not tabulated by Corliss and Sugar (1979). We could not find $3d^3(b^2F)4s\,^3F$, expected at ca. 24 kK (3.0eV) and both the singlet and triplet D terms based on $3d^3(d^2D1)4s$, and expected some 11.4 kK higher are missing. C. H. Corliss (1982) has remarked that this spectrum clearly needs a modern analysis.

Surveys of stellar spectra (Cowley 1978, Dworetsky et al. 1980) have revealed a small number of stars with extremely strong Co II lines. Some strong lines which were comparable in strength to Fe II λ4173.45 were not even in the Multiplet tables. We made the identifications with the help of the list by Velasco and Adames (1966) and unpublished work kindly made available by L. Iglesias. The list has subsequently been published (Iglesias 1979). However, some strong, unidentified features remain in these cobalt stars (see Adelman 1974), and the probability is good that further laboratory work on Co II will enable them to be identified.

Relatively little systematic identification work in the visual has been done on A stars, and the dispersions have typically been lower than those used in the photographic. The general situation is perhaps exemplified by the study of Little and Aller (1970) of the iron- and titanium-rich star HR 6870 (HD168733). The fraction of features that can be identified decreases markedly for wavelengths longer than λ4800. Some of the difficulty is due to the lower resolution (8A/mm in the visual, 2A/mm in the photographic), but incompleteness of laboratory data for common ions is a very likely cause. W. P. Bidelman (1982) has remarked that sources of laboratory wavelengths tend to run out in this region.

Investigations in the vacuum UV, now common in stellar spectroscopy, strongly tax existing tabulations, because relatively little laboratory work in this domain has been done. If we consider the energy of a photon at λ1000, 100 kK, we see that this energy is sufficient to lift all of the singly ionized iron-group ions from low levels well past the "top of the heap" where the levels have been well explored. It is no small wonder then, that astronomers who work with IUE spectra typically lament the inadequacy of the UV line lists (Adelman and Shore 1981, Dworetsky 1982).

III. Second and Third Spectra of Iron Group Elements

The structure of Fe II was recently studied by Johansson (1978). Table 3 is a sample of some of the configurations that are still missing in that spectrum.

Once the top of the heap (ca. 90-100 kK) is reached it becomes easy to find missing terms. Apart from the lower levels, which had been explicitly noted by Johansson, the remaining entries in the table may be regarded as sampling this domain. Recall that T_I is 130.6 kK.

Table 3

Sample Listing of Missing Terms in Fe II

Term or Configuration	Expected (kK)	Remark
$3d^6(^1S1)4s^2\,^2S$	60	Parent unknown in Fe III
$3d^6(^1D1)4s^2\,^2D$	60	Parent unknown in Fe III
$3d^54s^2\,^{2}2I, {}^2D, {}^2F$	68-74	
$3d^5(^4G)4s4p(^3P)^6H^0, {}^6G^0$	85	
$3d^5(^4P)4s4p(^3P)^6S^0$	90	
$3d^5(^2D2)4s^2\,^2D$	94	"Top of heap"
$3d^6(^3P2)5s\,^4P, {}^2P$	98	"Top of heap"
$3d^5(^2G1)4s^2\,^2G$	103	"Top of heap"

We have probed the following ions for an indication of the top of the heap: Sc II, Ti III, Cr II, Cr III, Mn II, Fe II, Fe III, Ni III. The ratio T_I/T_H ranges

from 2.7 Cr II to 1.2 in Sc II. A typical value is about 1.5. Except for Cr III, these are all ions where "further progress would be extremely difficult" (Cowan 1981). Nevertheless, we shall hear at this meeting from Johansson of fruitful work on Cr II and its applications to stellar spectroscopy.

IV. Second and Third Spectra of the Lanthanides

Martin et al. (1978) summarize analyses of the lanthanide rare earth elements (REE). Progress on second and third spectra since that publication has been slowed by shifting emphasis in research trends in atomic physics. What we can see from Martin et al. is that analyses of second spectra extend roughly halfway to the ionization limit, except for Yb II, where levels above the ionization limit are known. Thus, for the second spectra of the lanthanides we have T_I/T_S about 1.5 while in the iron-group elements T_I/T_H is typically 1.5.

The second spectra of FEE are fairly well represented in NBS Monograph 145 (Meggers, et al. 1975) as far as astronomical applications are concerned. The wavelengths are mostly classified for the even Z elements, but are rather poorly classified for those with odd Z.

A claimant astronomical need is the completion of line classifications, and derivation of precision oscillator strengths for some 50-100 lines in these spectra. Very useful work has been done by Maier and Whaling (1977), Lage and Whaling (1976), Karner et al. (1981), Anderson et al. (1975), and Arneson et al. (1977). We need slightly longer line lists and/or improved accuracy in order to derive useful oscillator strengths from the Monograph 145 data in the manner of Cowley (1982) and Cowley and Corliss (1982).

With the third spectra of the lanthanides we have reached the rough and ready frontiers of spectroscopic knowledge. Of the 15 spectra only La III, Ce III, and Lu III rate an A from Cowan. No levels at all appear in Martin et al. for Pm III or Dy III. Aikman et al. (1979) summarize surveys for these third spectra in CP stars, in many cases using unpublished material from Henry or Hannah Crosswhite, Meinders, or Sugar.

These third spectra are strongly present in some CP stars, and often they represent the dominant stage of ionization. Very strange abundances are inferred from the second spectra which are trace species, according to our models. We badly need term analyses and oscillator strengths.

We noted the following actinide spectra are present in HR 465 at its rare-earth maximum stage: U II, Th II, Th III (Cowley and Rice 1981). There is evidence for U II in a few other CP stars, and a careful search will undoubtedly dredge up evidence for thorium in some of these stars as well. We have continued our search for trans-uranic actinides (Cowley et al. 1976), but no positive results beyond those expected by chance have emerged.

V. Conclusions

Significant advances in atomic spectroscopy are urgently awaited by the astrophysicist. Perhaps as the full potential of modern digital processing and experimental techniques are brought to bear on these complex problems, we will experience a breakthrough in getting very detailed descriptions of atomic spectra necessary to model astronomical plasmas.

The astrophysical applications provide strong motivation for getting this machinery rolling. Rich scientific rewards await the researcher with the keys to an understanding of astronomical spectra.

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suggestions.

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