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High resolution ultraviolet spectroscopy from space observatories – what atomic physics and astrophysics can do for each other

ABSTRACT

Stellar spectra obtained with the IUE satellite demonstrate the complexity and richness in information of the 1150 -3300 A region. Ultraviolet astrophysical spectroscopy will reach a new plateau of resolution and precision with the launch of the Hubble Space Telescope in 1990. The atomic data base required for the accurate analysis of IUE and HST data lags well behind our observational capabilities in completeness and quality. We describe a project to assess the currently available atomic data, particularly for the lower ionization states of the iron-group and lighter elements. We illustrate the capabilities of the HST/GHRS instrument, and provide examples of transitions of special interest for early HST research.

INTRODUCTION

The sharp-lined, ultraviolet, photospheric absorption spectra of slowly rotating early-type stars contain a wealth of astrophysical information about the cosmic abundances of the elements and about physical processes occurring in the stellar surface layers. The effective temperature range 8500 K to about 20000 K encompasses young, normal A and B-type stars, a variety of chemically peculiar stars, and several types of very old, highly evolved stars. High resolution spectroscopy of these objects in the 1100 to 3000 A range provides access to lines of many atomic species not well represented in ground-based, optical spectra and to intrinsically strong resonance and low excitation lines which are often less susceptible to non-LTE effects than are their more highly excited congeners, observed at optical and near-infrared

wavelengths. These spectra are also a rich "laboratory" for the study of atomic spectra, particularly those of the first few ionization states of the iron group and lighter elements. The density of lines of observable strength is great (up to tens of lines per Angstrom) for reasons that are described by Johansson (1984). This creates both opportunities and problems: opportunities to obtain substantial new information about the atomic structure of many species, and problems in obtaining quantitatively accurate astrophysical information from the spectra, because of serious line blending and difficulties in locating the line-free continuum. Thus, ultraviolet spectrum synthesis is hindered by the compounding of three sources of uncertainty related to atomic data: 1. uncertainty in the wavelengths, oscillator strengths and broadening parameters of the primary lines being analysed; 2. uncertainty in the identity and atomic parameters of the lines with which the primary lines are blended; and 3. uncertainty in the position of the reference level relative to which absorption line strengths are measured, the continuum.

Fortunately, the massive, semi-empirical atomic data bases calculated originally by Kurucz and Peytremann (1975) and Kurucz (1981) have provided a rational starting point from which to attack these problems, converting UV spectrum synthesis from the hopeless to the very difficult. Over the past four years Kurucz has recomputed predicted energy levels, wavelengths, oscillator strengths and broadening parameters for the first nine ionization states of elements z = 20 to 28. His preliminary new data base for the first four ions of these elements, of greatest relevance here, now contains data for about 25 million predicted lines. However, only those lines involving transitions to experimentally determined levels have sufficiently accurate wavelengths to be used in spectrum synthesis. This limits the currently applicable data set to about half a million lines. The on-going term analysis of iron-group spectra by Johansson and others, based on laboratory observations, is the critical process which allows the conversion of lines from the predicted category to the "good" (i.e. accurate) category.

Good quality co-added stellar spectra obtained with the International Ultraviolet Explorer satellite at moderate resolution and signal-to-noise ($\lambda/\delta\lambda$ = 12000, S/N = 50,

Leckrone and Adelman, 1989) provide the opportunity to begin to assess the completeness and accuracy of the available atomic data base applicable to the ultraviolet. We report here the initial results of a detailed examination we have undertaken of the spectral content of the normal, A1 V star, omicron Pegasi (o Peg), in five test intervals within 1700 - 1900 A. We compare the IUE observations, line-by-line, with synthetic spectra, calculated using the new Kurucz data base, supplemented with data for the lighter elements from Kurucz and Peytremann and other sources. The match is good enough to indicate that we are on the right track, both observationally and computationally. Each specific discrepancy is then assessed in terms of the accuracy of energy levels and transition probabilities of the theoretically calculated lines, in terms of what is known from laboratory spectra, and in terms of phenomena of atomic physics, such as configuration interactions, which are difficult to predict theoretically.

With the launch of the Hubble Space Telescope (HST) and its Goddard High Resolution Spectrograph (GHRS) next year, UV astrophysical spectroscopy will undergo a quantum jump in precision and resolution ($\lambda/\delta\lambda = 25000$ to 90000; S/N up to 400 at the lower resolution and up to 80 at the higher). We illustrate in this paper the potential of the GHRS with examples of simulated stellar spectra at this resolution. Currently the state of the atomic data needed to quantitatively analyse GHRS (and IUE) data is lagging well behind our observational capabilities. We face the bleak prospect of attempting to analyse spectra of 1% precision, obtained at great expense, with atomic parameters that can be inaccurate by factors of 2 or 10, if they exist at all. The GHRS will be relentless in highlighting this problem. Two general types of activity are needed: continued development of the very large atomic data bases needed to accurately treat UV line blending and to synthesize wide spectral intervals for continuum placement; and determination of accurate wavelengths, oscillator strengths and broadening parameters for individual UV lines critical to specific astrophysical problems, examples of which are given here. In turn, atomic physics will reap a substantial benefit in terms of the feedback of information about the atomic structure of many species, including those difficult to observe in the laboratory.

ANALYSIS OF TEST INTERVALS IN o PEG SPECTRUM

We have selected five wavelength intervals 12 to 15 A wide for a detailed comparison between IUE observations and synthetic spectra calculated with the new Kurucz iron-group data base. These are listed in table 1. The "quality" designations A through D are very rough indicators of our expectations prior to the study about the completeness and quality of the atomic data within each interval. Currently, we have

Table 1. Test intervals for evaluation of quality and completeness of atomic data base

Wavelength (A)	Quality
1857 - 1872	B
1838 - 1851	A
1751 - 1765	D
1740 - 1752	C
1728 - 1741	C

completed the initial calculations and evaluations with respect to atomic physics for each interval. We have also iterated the calculations once to determine the effect of modifications made, on the basis of these evaluations, to log gf values and wavelengths and the effect of the addition of "new" lines omitted from the initial calculations. This work is still very much in progress, and several additional iterations of the calculations will be necessary before we are satisfied that all possibilities to improve the fit, based on current knowledge, have been exhausted. At that point, the remaining discrepancies between observations and calculations should give an indication of the work remaining to be done on the atomic data base in this wavelength region. Note that the calculations utilize a line-blanketed, LTE model atmosphere, abundances, and microturbulent velocity derived by Adelman (1988) in a very thorough ground-based study of this star. For elements for which the optical region abundances are poorly known, we adopt solar abundances. Some of the discrepancies we find in this comparative study may reflect errors in the assumed abundances, which will later be resolved by abundance work in the UV. In such cases, however, we would expect to find systematic discrepancies in many lines of the same element.

In the following discussion, we illustrate in detail the initial evaluation of one test interval, 1740 - 1752, and present selected results from several others. Figure 1 shows the observed spectrum and figure 2 the initial theoretical calculation, unaffected by instrumental broadening or by the broadening of lines due to the star's rotation. In figure 3 the theoretical spectrum has been broadened to the instrumental resolution of 0.15 A and to a projected stellar rotational velocity of 9 km s^{-1}. The latter is then superposed on the observed spectrum in figure 4. The N I and
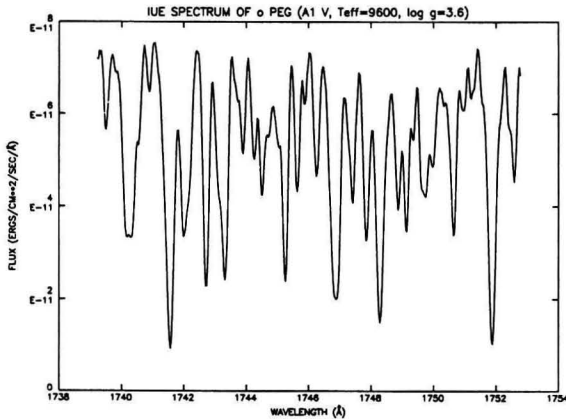
Fig. 1. IUE spectrum of o Peg, obtained by co-addition of nine large-aperture images.

C I lines labeled in figure 3 illustrate lines of particular astrophysical interest, which appear to be reasonably "clean" in the observations. (The N abundance has been adjusted to achieve a good fit, as part of another study, and in fact is about 0.5 dex below solar in these illustrations).

Inspection of figure 4 immediately shows a reasonably good match between calculation and observation for some absorption features, but also numerous examples of missing opacity and discrepant line strengths. The line-by-line investigation of each disparity between observation and calculation revealed three general classes of problems in all the test intervals: missing lines; apparent
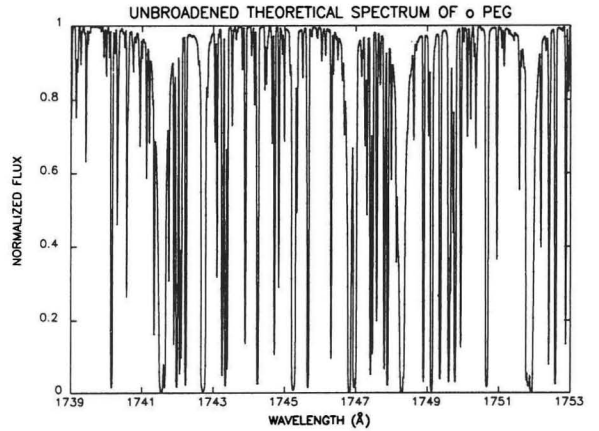

Fig. 2. Theoretical spectrum for o Peg, calculated with new Kurucz atomic data.
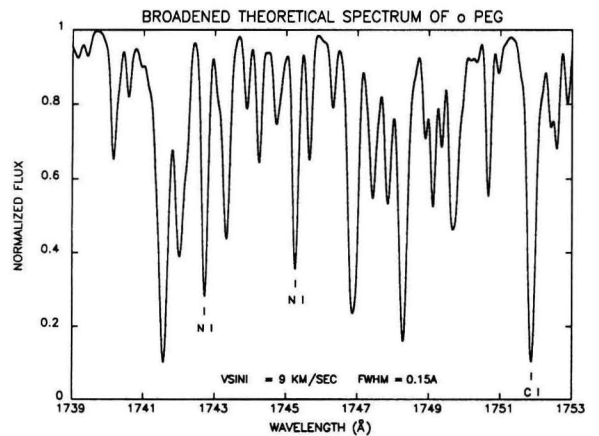

Fig. 3. Theoretical spectrum of figure 2, convolved with instrumental broadening and stellar rotational broadening functions.

discrepancies in the Kurucz oscillator strengths or wavelengths with respect to line strengths or wavelengths observed in laboratory data; and some very interesting examples of the effects of level mixing.
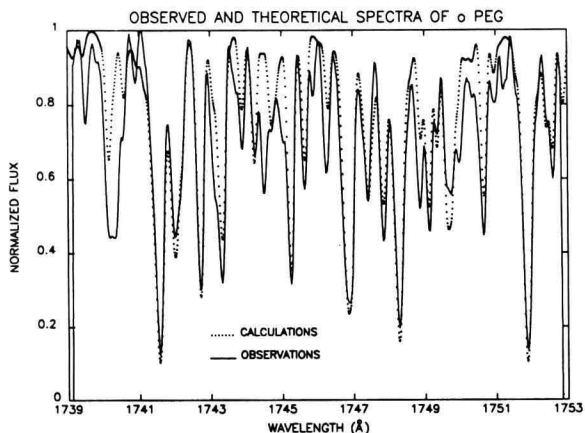
Fig. 4. Observed spectrum normalized to the estimated position of the line-free continuum and superposed on the theoretical spectrum of figure 3.

Lines Missing From The Atomic Data Base

Figure 5 shows a 4 A subsection of a test interval with the positions marked of 15 lines which did not appear in the original set of "good" Kurucz lines and were, therefore not contained in the original calculation. Those labeled "new FeII" are lines found in the set of predicted Kurucz lines, arising in transitions to upper levels which Johansson has recently identified from experimental term analysis. Their wavelengths are now known with good accuracy and Kurucz has already calculated their oscillator strengths and damping parameters, so that they could be included in the first iteration of the spectrum synthesis, labeled "revised calculation" in figure 5. Lines labeled "new FeI" have also been identified in laboratory spectra and their lower level excitation potentials are known. However, we can only estimate their log gf values by similarity to other FeI lines of similar strength. Those rough estimates will be refined in subsequent iterations. The numerous lines labeled "unk" (an abbreviation of "unknown") in figure 5 are known to exist in laboratory spectra of the denoted element, although the ionization state is not always known with certainty. Since their excitation potentials and oscillator strengths are presently not known, they could not be included in the revised calculation. It is encouraging that these "unk" lines correspond in several cases to positions where line opacity is clearly missing from the calculations, suggesting

possible identifications for the missing lines. It is also gratifying that several of the "new" lines added to the calculation clearly improved the match to the observations.
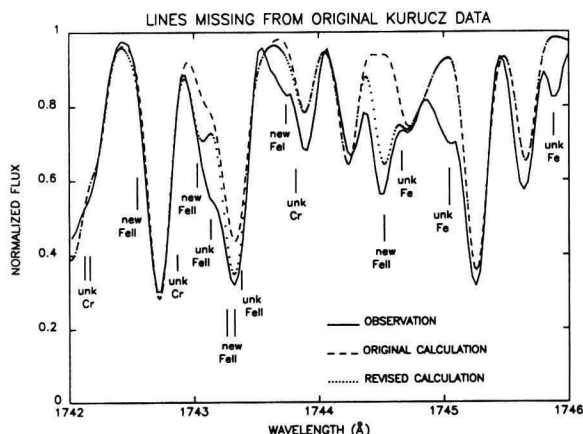

Fig. 5. Examples of lines seen in laboratory spectra which were not included in the original calculation.

"Discrepancies" In The Atomic Data Base

A segment of the 1858 - 1870 test interval shown in figure 6 illustrates the situation where there are apparent disagreements between the relative strengths of lines of similar excitation seen in laboratory spectra and the relative strengths one would infer from Kurucz's log gf values. For example, two FeI lines at 1863.548 and 1865.309 A (labeled "stronger in lab." in figure 6) have calculated log gf's -3.11 and -3.71, respectively. These lines, arising from 0.00 eV, are seen in absorption in laboratory spectra with a strength comparable to other FeI lines for which Kurucz has calculated larger log gf's. Our initial estimate was that log gf for 1863.548 should be in the range -1.5 to -2, while that for 1865.309 should be near -1.0 to -1.5. In both cases the substitution of log gf's in our revised calculation resulted in lines that are stronger than observed in the stellar spectrum. Further iterations will allow us to test how "discrepant" the Kurucz log gf's might be. One expects the calculated log gf's for FeI to have rather large uncertainties because of its complex atomic structure, which has many interacting series converging towards the lowest limit. The majority of FeI lines below 2000 A are unclassified, and the levels from which they arise are unknown.

Thus, stellar and laboratory absorption spectra should, in principle, be especially useful in establishing the relative strengths of FeI lines in the far UV.
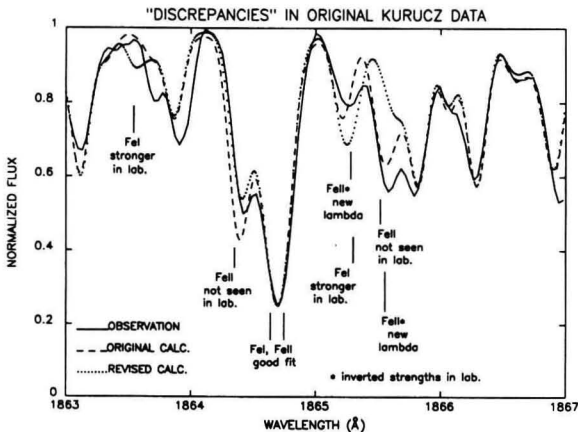

Fig. 6. Examples of apparent "discrepancies" between the Kurucz atomic data base and laboratory data.

Two FeII lines, at 1864.357 and 1865.530 A, are not seen in laboratory spectra, although with the excitation potentials and log gf's given by Kurucz (E.P. = 2.34 and 2.28 eV; log gf = -3.25 and -2.75, respectively) they are calculated to be moderately strong lines in o Peg. The 1864.357 A line is observed to be weaker than calculated in the stellar spectrum (figure 6). Eliminating the line entirely from the synthetic spectrum, as illustrated in the revised calculation, is clearly going too far. A more accurate log gf for this line should be obtainable from further iterations of the spectrum synthesis. Such a refinement of log gf may not be possible for the 1865.530 A line, since it is unresolved in these observations from another FeII line, 1865.545 A, which also has a serious problem, discussed below.

Two FeII lines, at 1865.212 and 1865.545 A, arise from the same upper level and have wavelengths given by Kurucz (1865.221 and 1865.554 A, respectively) that we have revised slightly due to a small revision in the experimental level value. More significantly, in the laboratory data 1865.545 is stronger than 1865.212. The reverse is true in Kurucz's log gf's (-0.65 for 1865.212, -1.83 for 1865.545). We have not attempted to modify the log gf's in the revised calculation in figure 6. The

discrepancies in these log gf's, together with unresolved blending with the other problematical lines discussed previously, results in the poor fit to the observed profiles of these lines illustrated. It will require the resolution of the HST/GHRS to disentangle the blended lines and to obtain further astrophysical information about their relative strengths.

To conclude this discussion of examples of "discrepancies" in the Kurucz atomic data base, we note that the observed feature at 1864.70 A, a blend of two FeII lines and one FeI line, is already rather well fit by the original calculations, using the Kurucz data as given. Clearly, the Cowan (1968) code used by Kurucz is capable of providing accurate data, limited primarily by the quality of the input energy level information and by the knowledge of configuration interactions.

Problems of atomic physics

The most remarkable spectral interval that we have investigated is illustrated in the sequence of figures 7 through 9. There are two (and perhaps three) different examples of interesting phenomena of atomic physics affecting the spectrum synthesis here. Figure 7 illustrates the initial calculation. We note that, from 1857 to 1869 A, the computational match to the observations is as good as, or better than, that in any other of the test intervals, with occasional
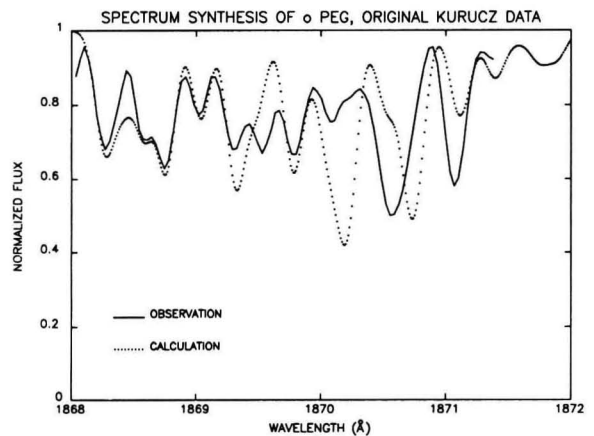

Fig. 7. Initial calculation for a portion of the 1857 - 1872 A test interval.

instances of missing line opacity and other discrepancies as discussed previously. But

from about 1869.1 to about 1871.2 A the quality of the spectrum synthesis becomes especially bad. In iterating the calculation, we first introduced "new" FeI lines at 1869.260 and 1870.352 A, with roughly estimated log gf's, based on relative laboratory intensities. Four "new" FeII lines were added at 1869.553, 1870.534, 1871.004 and 1871.056 A. Only the first of these has a known Kurucz log gf. Classification of the other three FeII lines is not complete, and estimated log gf's were also adopted for them. These lines are labeled in figure 8. Also shown are the positions of four SiII lines, belonging to multiplet UV 9.02, the lower, $3s3p^2$ ^2D, term of which is known to strongly interact with $3s^23d$ ^2D (Froese Fischer, 1968; Artru, et al., 1981). Since Kurucz and Peytremann did not include this configuration interaction in their calculations, their log gf's for these SiII lines are in error by about 2 dex (Lanz and Artru, 1985). Therefore, we substituted the SiII log gf's from Artru, et al., in the revised calculation shown in figure 8.

The quality of the fit between observation and calculation in figure 8 is somewhat better than in figure 7. However, several serious discrepancies remain. Of particular interest is the observed feature at 1870.6 A. In addition to the "new" FeII line,
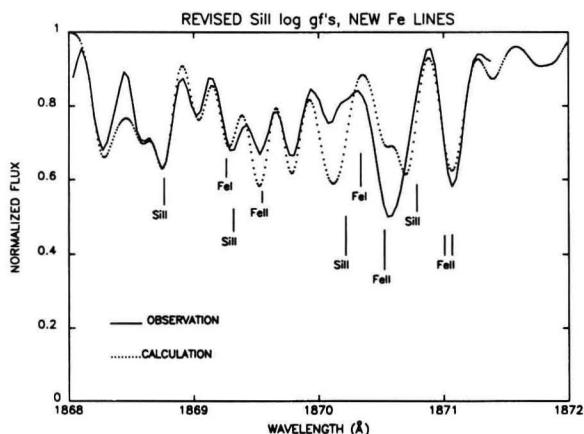
Fig. 8. Spectrum synthesis including "new" Fe lines and SiII log gf's which take account of configuration interactions.

1870.534 A, mentioned previously, two other FeII lines found in the Kurucz data base contribute to this feature - 1870.607 A (b^2P - x^6P) and 1870.697 A (b^2P - w^2P). In the

1950's Edlen found that the accidental coincidence of these two upper levels, separated by 2.4 cm^{-1}, results in a strong mixing between them, even though they are otherwise completely unrelated (Johansson, 1984). If we assume a 50-50 mixture, then the original Kurucz log gf's, -6.50 and -1.76, respectively, become -2.10 for both lines. Substituting this value into the calculation results in the synthetic profile plotted in figure 9. Clearly, the qualitative shape of the calculated profile now more closely resembles the observed profile than in figures 7 and 8. Further adjustments to the total gf-value for the combined transitions, 1870.607 and 1870.697, as well as adjustments to the originally estimated log gf for the "new" FeII line at 1870.534 A might yield an acceptable match to both the shape and strength of the observed feature. However, the preferred course is to attempt to resolve these components with the HST/GHRS.
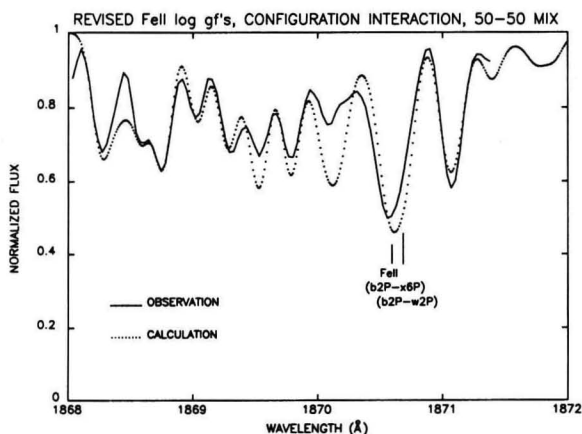
Fig. 9. Spectrum synthesis accounting for mixing due to accidental coincidence of FeII upper levels.

In general, theoretical calculations are not sufficiently accurate to reliably predict mixing due to the accidental coincidence of levels. Laboratory and astrophysical data are essential in finding and evaluating short-range effects of this kind in complex spectra.

One remaining concern about the spectrum synthesis shown in figure 9 is the grossly excessive absorption predicted at 1870.1 A. A major contributor to the feature is FeII 1870.169 A, about which there is a mystery. This line, which in LS coupling should be one

of the strongest members of its multiplet, 4s a^{4}D-4p y^{4}F, does not appear at this wavelength in laboratory spectra, but rather another component of the same multiplet, predicted by Kurucz to have a log gf value two orders of magnitude less. From both the calculated log gf's and the relative laboratory intensities for all the lines in the multiplet, we know that LS relative intensities do not apply. Moreover, the agreement between relative calculated log gf's and relative laboratory strengths for many of the lines in the multiplet is not good. Johansson notes that several lines in the multiplet, though not 1870.169, have different log gf's in the new Kurucz calculations than in Kurucz (1981), suggesting that new configuration interactions were included in the more recent calculations. But the configuration interactions directly relevant to this multiplet were included in 1981. He speculates that mixing in the theoretical calculations between the ^{4}F upper term of this multiplet and a higher lying ^{4}F term of the same parent configuration may result in changes in predicted log gf's for this multiplet, if the higher lying ^{4}F term is perturbed by newly included configuration interactions. The simple question for atomic theorists is, is this mixing between terms having the same type of LS parent term (3d^6^{3}F in FeIII) correct or not? The next iteration of our calculations will utilise a log gf = -5.5, rather than the value, -3.64, listed at this wavelength by Kurucz.

We conclude the discussion of the assessment of the test intervals, by illustrating in figure 10 the current theoretical fit (after one iteration) to the observations in our "A-quality" interval, 1838 - 1851. Here the qualitative match to the shapes of some obviously complex blends is remarkably good, and there are numerous features which we come close to matching in absolute quantitative terms as well. On the other hand, even in this the best interval, there are still examples of missing line opacity, discrepancies in line strengths and perhaps even anomalies in transition wavelengths. Note for example the good fit to the detailed profile of the complex feature near 1846.7 A, while next to it, at 1846.0 A, is another blend for which the fit is strangely poor. It is clear from this exercise that the information content of these spectra is high, from both an astrophysical and an atomic physics viewpoint. It will be much higher still in
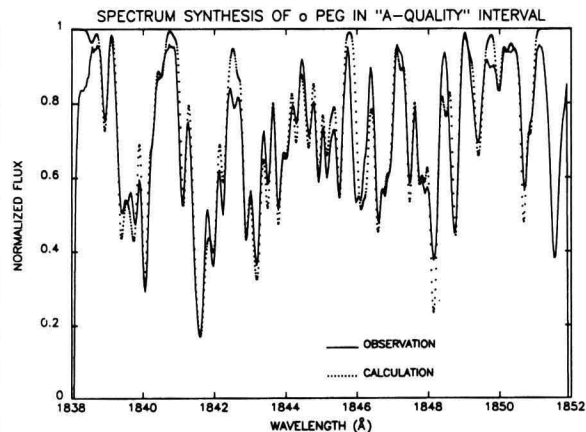

Fig. 10. First iteration of spectrum synthesis of test interval in which atomic data were expected to be relatively complete.

the HST/GHRS spectra.

OBSERVATIONAL CAPABILITIES OF THE GHRS

The GHRS, scheduled to be launched on the HST in 1990, will be photometrically superior to the IUE, as well as capable of higher spectral resolution. With its 512-diode digicon detectors, it will provide a highly linear photon counting capability over a very wide dynamic range. Its chief shortcoming will be the time required to cover wide spectral intervals with its one-dimensional detector arrays. In the high resolution mode it will measure wavelength intervals ranging from 5 to 16 A in a single observation. In the IUE observations of o Peg illustrated in this paper, the primary determinant of spectral resolution is the resolving power of the instrument. In GHRS observations of sharp-lined stars, resolution will be limited primarily by the doppler broadening of spectral lines by stellar rotation. For o Peg we have adopted a projected rotational velocity vsini = 9 km s^{-1} (it may actually be a bit lower). Other early-type stars, especially in the chemically peculiar HgMn sequence, have unmeasurably small rotational velocities and will appear exceedingly sharp-lined in GHRS data. Figure 11 shows a five angstrom segment of the theoretical spectrum of o Peg, broadened to the resolution of the IUE. In figure 12 we show the spectrum as it might appear in data obtained with the GHRS, assuming the stellar vsini = 9 km s^{-1}. For a similar star with slower projected rotation

(either because the star is intrinsically slowly rotating or because it is seen pole-on), the spectrum might appear as shown in figure 13. Ambiguities and quantitative inaccuracies in spectrum syntheses, caused by unresolved blending, will at least be improved, if not remedied, by data of this quality. Moreover, one will be able to
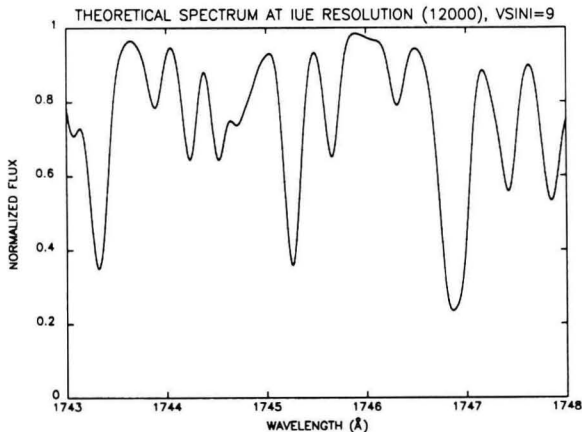

Fig. 11. Calculated o Peg spectrum broadened to the resolution of the IUE.

resolve closely spaced lines, whose relative strengths need to be accurately measured, such as the FeII 1870.607 and 1870.697 A lines discussed previously. Astrophysicists will need atomic data of quality commensurate with the quality of these observations. This
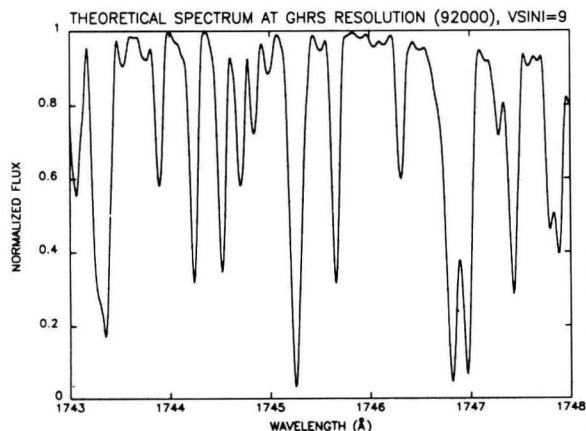

Fig. 12. The same spectrum as in figure 11, broadened to the resolution of the GHRS.

means an atomic data base which is essentially complete with respect to the stronger transitions in the first four ionization states of the more abundant elements, with well determined wavelengths, and log gf values that are accurate to at least 0.1 dex. The process of creating such a data base, however, will be an interactive one, involving direct working relationships among experimental and theoretical atomic physicists and spectroscopic astrophysicists.
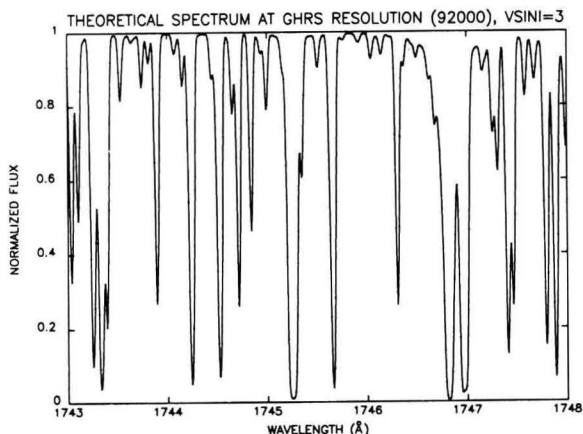

Fig. 13. The same spectrum as in figure 12 with reduced stellar rotation.

NEEDS FOR PRIMARY ATOMIC DATA

Two classes of accurate atomic data are needed for the quantitative analysis of ultraviolet stellar spectra. If we are attempting to derive the abundance of an element from specific, well observed lines, we need wavelengths, oscillator strengths and broadening parameters for those lines. We denote these as "primary" data. Of nearly equal importance, however, are a complete knowledge of what lines of other elements, or what weaker lines of the same element, are contributing significant opacity to the primary line and accurate atomic data for those blending contaminants. We denote these as "secondary" data. Our previous discussion has focused on the large atomic data base needed as the source of secondary data. Here we briefly describe some specific examples of primary data that are needed for the analysis of our own HST/GHRS and IUE data.

N I

A substantial literature exists about the spectrum and oscillator strengths of N I. In a study just completed, Roby, Leckrone and Adelman (1989, in preparation) used IUE spectra (including that of o Peg, illustrated in this paper) to derive nitrogen abundances from the multiplets near 1742.7, 1745.2 and 1411.9 A. When the experimental log gf values were used (e.g. from Wiese et al., 1966, renormalized according to Lawrence and Savage, 1966, or from Dumont et al., 1974) a systematic difference of 0.5 to 1.2 dex was found between abundances from the 1411 A feature and those from 1742 and 1745 A. The situation is complicated by the usual uncertainties in the background blending, which we have treated as carefully as possible.(We believe the random uncertainty in the abundance from a single line to be about ±0.3 dex.) Interestingly, this systematic discrepancy was greatly reduced or went away entirely when we adopted the calculated N I log gf's from Kurucz and Peytremann. Since all recently published oscillator strengths for 1742 and 1745 A, both theoretical and experimental, agree to within 0.1 dex, this result suggests that there is a problem with the expermental log gf's for the lines near 1411. The resolution of this discrepancy is very important, because the astrophysical interpretation hinges on which N abundance we adopt. The 1742/1745 abundances are below solar and below the values derived from high-excitation near infrared lines, while the 1411 values are close to solar and to the near-IR values. On the other hand we view the 1742/1745 abundances as the more reliable and have a ready astrophysical explanation for the disagreement with the near-IR values and solar values.

O I

We have attempted to derive stellar oxygen abundances from the low excitation intersystem lines of O I at 1356, 1359 and 1641 A. Oxygen lines observed in the red or near-IR are either very weak or are susceptible to large non-LTE effects. The lines of the oxygen resonance multiplet, 1302, 1305 and 1306 A, are broad, strongly saturated and difficult to measure accurately in our IUE data. Leckrone and Adelman (1986) reported a preliminary, and somewhat controversial, oxygen abundance for the highly evolved, horizontal branch star HD109995, based on the 1356 A line. But the literature is somewhat ambiguous about whether the log gf for this line from Zeippen, et al. (1977) or from Froese Fischer (1987) should be viewed as the more reliable (they differ by 0.5 dex, an astrophysically critical uncertainty). Moreover, Zeippen et al. did not compute a gf value for the 1641 A transition, a project that would be of great interest for the interpretation of IUE and GHRS observations.

Hg I, II, III, and Au II

Lines of the first three Hg ions will be extensively studied in GHRS spectra of the Hg-rich chemically peculiar stars. These stars exhibit isotope anomalies - the hotter members of the group having a terrestrial isotope mixture and the cooler members being deficient in the lighter Hg isotopes (the Hg lines in the most extreme case, the star chi Lupi, arise from nearly pure ^{204}Hg). The only astrophysical model currently offered to explain this anomaly invokes the diffusion of the lighter isotopes to high stellar atmospheric layers, where they "hide" in the form of Hg III. To test this hypothesis, one has to search for the Hg III lines in the ultraviolet, and hopefully measure abundances from them. They have not been found in IUE spectra. But we do not know their oscillator strengths and cannot predict how strong they should be. Similarly, one wants to measure abundances using lines of Hg I and Hg II for comparison. In a related area, GHRS will be

Table 2. Lines of Hg and Au for which oscillator strengths are needed

Ion	Wavelength (A)
Hg I	2537
	1849
Hg II	1942
	1650
Hg III	2354
	1678
	1379
	1335
	1331
Au II	2082
	1801
	1783
	1740

used to look for ultraviolet lines of Au II in these stars, searching for the abundance pattern as a function of atomic number (the stars are often Pt-rich as well). Extremely weak Au lines have been detected in two or three stars in ground-based spectra, but one would get more positive detections and more accurate abundances from ultraviolet lines. Table 2 lists the Hg and Au lines that we are planning to observe with the GHRS.

ACKNOWLEDGEMENTS

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