Atomic data for stellar astrophysics: from the UV to the IR[1]

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Abstract: The study of stars and stellar evolution relies heavily on the analysis of stellar spectra. The need for atomic line data from the ultraviolet (UV) to the infrared (IR) regions is greater now than ever. In the past twenty years, the time since the launch of the Hubble Space Telescope, great progress has been made in acquiring atomic data for UV transitions. The optical wavelength region, now expanded by progress in detector technology, continues to provide motivation for new atomic data. In addition, investments in new instrumentation for ground-based and space observatories has lead to the availability of high-quality spectra at IR wavelengths, where the need for atomic data is most critical. In this review, examples are provided of the progress made in generating atomic data for stellar studies, with a look to the future for addressing the accuracy and completeness of atomic data for anticipated needs.

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Résumé : L'étude des étoiles et de leur évolution repose largement sur l'analyse des spectres stellaires. Le besoin de données sur les raies atomiques, de l'ultraviolet jusqu'à l'infrarouge, n'a jamais été plus grand. Ces vingt dernières années, depuis le lancement de Hubble, des progrès importants ont été faits dans l'étude des transitions atomiques dans l'ultraviolet. La région des longueurs d'onde optiques est maintenant agrandie grâce aux progrès en technologie de détection et ses données spectrales atomiques demeurent d'un grand intérêt. De plus, les investissements dans des instruments nouveaux, basés sur Terre et dans l'espace, ont rendu possible l'obtention de spectres de très grande qualité dans l'infrarouge, là où le besoin en données est le plus criant. Nous passons ici en revue des exemples de progrès faits pour générer les spectres requis en études stellaires, gardant un œil sur l'avenir et ses besoins en précision et complétude des données atomiques pour les besoins à venir.

[Traduit par la Rédaction]

1. Introduction

The application of laboratory spectroscopy to the analysis of stellar spectra dates back nearly two centuries, to a time when nascent studies of the solar spectrum provided motivation for laboratory work. The comparison of early laboratory techniques [1] with those of the present day give a familiar feeling in principle and, to some extent, practice. The laboratory studies of the late 1800s were published in specially established journals, first *Astronomy and Astro-Physics* and then *The Astrophysical Journal*, which were envisioned to serve as a reservoir of laboratory astrophysics results [2] in an age when deep-sky photography and stellar kinematics were popular. These early studies at optical and near-ultraviolet (near-UV) wavelengths have since been extended towards both ends of the electromagnetic spectrum. The symbiosis that exists between laboratory spectroscopy and astronomy is such that stellar spectra are utilized to investigate topics in spectroscopy because astronomical environments are difficult to replicate in the laboratory (cf. [3], on 4d–4f Fe II transitions). Stellar spectra are, therefore, not to be considered an exotic entity relegated solely to the astronomer to decipher. Instead, these self-gravitating plasma spheres present conditions that extend the study of plasmas to more extreme conditions than are currently created in laboratories.

As a foreword to the topic of atomic data for stellar spectrum analysis, let us consider properties of stars and their spectra. As was recognized by astronomers in the late 1800s, the taxonomy of stellar spectra showed that stars presented a range of spectrum characteristics, which reflected the physical conditions. The Harvard College Observatory classification system [4, 5], which was the precursor to the current MK classification scheme [6], was arranged to be a temperature scale, and certain spectral lines provided a separation in luminosity, which was introduced as a second spectral parameter. Luminosity became synonymous with stellar surface gravity, which is associated with gas pressure. The effective temperature–luminosity (T_{eff}–L) diagram, a variant of the H–R diagram, named after Eijnar Hertzsprung and Henry Norris Russell for their work one century ago, is now a cornerstone of stellar astronomy.[2]

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[2]T_{eff} is an indicator of stellar photospheric temperature, related to flux per unit area on the star $F = \sigma T^4_{eff}$, while luminosity is the surface-integrated flux $L = 4\pi R2\sigma T^4_{eff}$.

Through stellar spectral classification, it is possible to identify peculiarities from established standards. Since stars spend most of their existence (excluding their final end-state) transmuting hydrogen into helium on what is termed the *main-sequence* strip of the H–R diagram, their surface composition represents the pre-stellar cloud chemical composition from which they were formed. This birth composition has changed over the history of the Galaxy, as heavy elements have been created and dispersed throughout the interstellar medium (ISM). Since low-mass stars ($M < 0.8$ $M_\odot$) have main-sequence lifetimes at least as long as the age of the Galaxy, we observe stars over this age range, and their stellar spectra reflect the corresponding range in their birth chemical composition.

In addition to this long-term evolution in chemical composition, individual stars more massive than approximately 80% of the Sun's mass, cycle through various nucleosynthesis processes in their core regions after their main-sequence phase. For many stars, these comparatively short time-scale processes create heavy atoms that are dredged up to the photosphere by convective currents. We detect the presence of processed material by spectral line variations with respect to the main-sequence stars of similar mass and age. When these stars occur in close binary star systems, the giant star can transfer material to its companion, thereby polluting its atmosphere and changing its spectral signature.

A third process that can produce nonstandard surface chemical compositions and spectral peculiarities is atomic diffusion within the atmospheric and sub-atmospheric (envelope) regions of warm stars, as put forward by Michaud et al. [7]. For all stars there exists a region where the outwardly directed radiation pressure is in a fine balance with inwardly directed gravity. A region of stability is established, relatively free from the mixing effects of turbulent or convective motions. One result is that certain atoms and (or) ions will be levitated in the atmosphere, perhaps even being expelled altogether, while others fall to depths below the continuum-producing layer, and thus out of view. The most well-known of this type of abundance peculiarity is represented by the warm magnetic stars, but high-resolution spectroscopy has identified chemical peculiarity among a large fraction of stars of spectral type B through A ($T_{\mathrm{eff}} \sim 20\,000$ to $8\,000$ K).

The lesson to be taken from this is that not all stars in our Galaxy present similar spectra. Chemical compositions may vary for several reasons, and the atomic data needs are not the same for all stars. In the discussion that follows, the intention is to show where atomic data are needed, which may serve to initiate work in these areas. Stellar astrophysics is the main driver for this discussion, because there exist a variety of stars that show the requisite sharp-lined spectra necessary to test atomic data. The analysis of the spectra of galaxies and more rapidly rotating stars naturally benefit from more accurate atomic data and may even be the impetus for acquiring more accurate wavelengths and oscillator strengths.

2. Defining the necessary atomic data

For this discussion, we first consider atomic data needed to describe absorption line profiles in stellar photospheres. The line profile, the wavelength dependent intensity I_λ, in a simple slab model atmosphere can be expressed as,

$$I_\lambda = I_0 \exp(-\tau_\lambda) \tag{1}$$

where I_0 is the continuum, or line-free intensity level.

For simplicity, the optical depth τ_λ can be separated into discrete (spectral line) l_λ, and continuous κ_λ components,

$$\tau_\lambda = l_\lambda + \kappa_\lambda \tag{2}$$

The line absorption coefficient is given by

$$l_\lambda = \lambda_{ij}^2 f_{ij} (N_i / N_{\mathrm{total}}) V \tag{3}$$

where λ_{ij} is the transition wavelength between lower level i and upper level j, f_{ij} is the oscillator strength, N_i/N_{total} is the ratio of the number density of the particles forming the line to the total number for the element, and V is the normalized line profile (Voigt profile). Within N_i/N_{total} are the Saha and Boltzman equations and the parameters of transition energy E_{ij}, ionization potential IP, statistical weight g, and the related partition function.

The laboratory spectroscopist, using emission line spectra, is able to measure line intensity, position, and shape. Experiments measuring the atomic energy level lifetimes (for example, by laser and beam-foil techniques) may also be capable of measuring relative line intensities. From these measurements, E_{ij}, IP, g, transition probability A_{ij}, angular momentum quantum number J, and branching fraction, $\mathrm{BF}_{ij} = I_{ij}/\Sigma I_j$, can be derived. In the stellar photosphere, particle collisions dominate over radiation for populating energy levels, and this is referred to as local thermodynamic equilibrium (LTE). (For non-LTE analysis the collision strengths for excitation and ionization of various species along with photoionization cross-sections are also needed to compute the populations of electronic states.)

The atomic states (neutral and (or) ionic) that can be studied in a stellar spectrum depend on T_{eff}. Typically, no more than three consecutive states will be detected from a photosphere. The presence of additional or discrepant ionic species is then likely due to multiple temperature regimes or specific processes, such as a binary star system or the detection of both the lower temperature photosphere along with higher temperature chromospheric or coronal plasmas.

Large data sets for spectral-line parameters for astrophysics date back to the work of Corliss and Bozman [8], who compiled wavelengths and oscillator strengths for 25 000 spectral lines of 70 elements over the wavelength interval 200 to 900 nm. These data are still used today for many lines that have not been re-analyzed, but have been noted by various researchers as having systematic errors. Another large data set is the MIT Wavelength Tables [9], which includes intensities for over 100 000 lines between 200 and 1000 nm. Large data sets have also been created from extensive calculations, such as those by [10, 11], and the MCHF/MCDHF Database [12]. The literature contains many studies for atomic data from experiment and calculation. However, there exists no single compilation that incorporates the best values for all lines. The Vienna Atomic Line Database (VALD) [13] is often used by astronomers in lieu of the Kurucz data set, but continuing work by Kurucz and others makes it challenging to keep compilations up to date. Bibliographic databases, including those from NIST [14] and Troitsk [15], along with the International Astronomical Union's Commission 14 (Atomic and Molecular Data) triennial report, are useful for locating new references, in addition to electronic search engines. Other large calculation-based atomic data sets are typically not considered by astronomers, although smaller directed studies, concentrating on specific lines or an ion, are common in the astronomical literature.

The question is inevitably raised regarding the relative importance of the completeness of the data set versus its accuracy. The solution to this dichotomy currently rests with the intended usage of the data. Completeness is most often the purview of opacity calculations, for which the inclusion of a multitude of extremely weak spectral lines has important consequences, and therefore higher uncertainties in wavelength and oscillator strength can be tolerated because of the inherent averaging process of the analysis. High accuracy is a priority for "fine" analysis of the spectrum, for which line selection may be limited by line blending or limited wavelength coverage.[3] Ultimately, we desire databases which will be both complete and highly accurate.

For this discussion, low resolution is defined as being sufficient for recording spectral energy distributions (SEDs) and measuring strong spectral features, such as the lines of the H Balmer series, He I, Ca II H and K, groups of metallic lines and molecular features (band-head positions and depths). An upper limit to the resolving power is approximately $R = 1000$, which is smaller than the resolving power established for MK stellar classification. A moderate resolution allows element abundances to be determined from individual spectral lines. The results of such an analysis depend on line blending (due to stellar rotation, spectral resolution, overall metallicity, and line density). The term "high-spectral resolution" is reserved for data capable of being analysed for the effects of atomic processes in spectral lines, including hyperfine structure (HFS), isotope shift (IS) and mixture, and magnetic broadening, and certain stellar atmospheric phenomena, including convective motion line asymmetries and highly precise radial velocity measurements. Excluding extreme examples of these phenomena, a resolving power of $R > 80\,000$, or roughly better than 50 mÅ resolution at optical wavelengths, is required.

High-resolution laboratory spectroscopy, conducted with Fourier-transform spectrometers, long focal length instruments and laser techniques, satisfies the high-resolution requirements of stellar spectroscopy, which have an ultimate resolving power limitation imposed by stellar rotation and (or) turbulent motions. (A caveat to this statement is that a star's entire visible hemisphere is observed, with the exception of the sun. Future instruments may be capable of high spatial resolution, which will allow spectra to be taken at different locations on the stellar surface (for nearby stars), thus removing the limitation on effective resolution from stellar rotation and possibly turbulence.)

3. A near UV catastrophe

The (UV) spectral region, defined here as the combined wavelength ranges of the Far Ultraviolet Spectroscopic Explorer (FUSE, 800–1175 Å), and instruments onboard the satellites International Ultraviolet Explorer (IUE) and the Hubble Space Telescope (HST) (1200–3200 Å), has proven to be critical for all aspects of stellar evolution studies. Stars of all temperatures have spectrum diagnostics in this region. Hot stars, spectral types O and B ($T_{\text{eff}} \sim 30\,000$–$10\,000$ K), have a prominant black-body-like continuum, on which absorption lines of excited atoms in the stellar atmosphere, along with interstellar lines of low ionization species, are superimposed. For warm stars, spectral types mid-B through A ($T_{\text{eff}} \sim 15\,000$–$7\,000$ K), the presence of atomic absorption lines from the lowest three spectra of many elements can be investigated. Finally for cool stars, spectral types F through M, a diminishing continuum yields to a rise in metallic emission lines from the chromosphere. These lines originate mostly from singly-ionized iron-group elements, reflecting a temperature of $(1–2) \times 10^4$ K. The signature of even higher energy processes, such as colliding winds, is evident from emission lines of high-excitation species, such as He II, C IV, N V, and O VI, across the full range of T_{eff}.

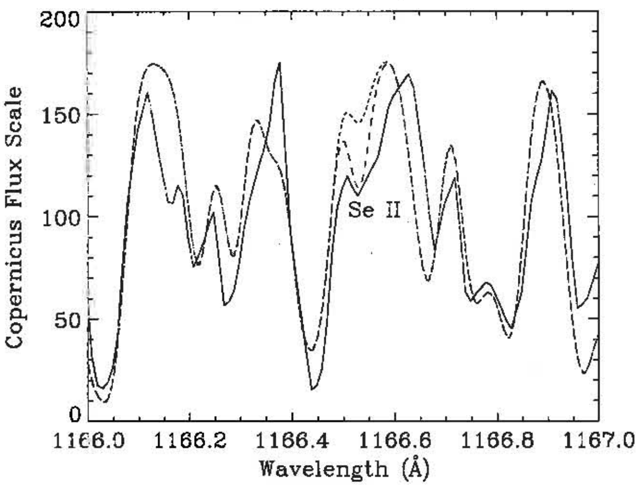
The first UV spectra for a large number of stars were obtained in the early 1970s by the Copernicus orbiting observatory. Its remarkable spectra, taken at a rather high spectral resolving power ($R \sim 30\,000$), remain a valuable resource of bright star UV spectra. Follow-up missions, IUE (1978–1996) and HST (1990 to the present) have provided continuous spectral capabilities in the 1200–3200 Å region for over 30 years, which has allowed astronomers to collect spectral data for targets of various types, perform follow-up studies, and conduct long-term monitoring. Far-UV access was provided by satellites, starting with Copernicus (1972–1981), a series of small missions (including the ASTRO and ORPHEUS platforms on the NASA Space Transportation System or Space Shuttle), and FUSE (1999–2007). The current HST Cosmic Origins Spectrograph (COS) has a limited capability for FUV spectroscopy.

The continuous history of UV spectroscopy, over 40 years, appears to be ending with the HST, as there is no planned NASA or ESA mission for the UV. Despite the anticipated hiatus of future UV missions, the legacy of completed and current missions is an extensive collection of spectra available through open-access archives. For the purposes of atomic spectroscopists and theoreticians, these archives provide a tremendous resource and motivation for continued analyses of atomic data. Additional atomic data are necessary for extracting further scientific results from stellar spectra that were often obtained for a singular purpose. Both the accuracy and completeness of the atomic data set for the UV are remarkably low, in particular for elements beyond the iron group.

An example of the concern over accuracy is presented in Fig. 1, a 1 Å segment of the Copernicus spectrum of the hot star 3 Cen A (B5 IIIp). Lines from the element selenium were searched by the author, with no positive identification of any Se II or Se III line being made. An earlier claim of Se II 1177 Å [17] in this stellar spectrum has not been confirmed by the author, using synthetic spectrum analysis. For the Se II 1166 Å line in Fig. 1, the oscillator strength is of particular concern to the identification. The calculated, and reportedly uncertain, *gf*-value of –0.32 [16], when used in

[3]Fine analysis was a common term used to define an analysis of individual spectral lines for abundance studies.

Fig. 1. A segment of the Copernicus spectrum for the star 3 Cen A (B5 IIIp) is compared with two synthetic spectrum calculations. The abundance of selenium is kept at the solar system level, while the *gf*-value for the Se II λ 1166.5 line is –0.32 (dotted line, from [16]) and +0.30 (dashed line, best fit).



conjunction with the solar-system selenium abundance, does not produce enough absorption. A best fit to the spectrum can be attained by either increasing the *gf*-value to +0.30 or increase the selenium abundance by a factor of four, provided that unidentified lines of significant strength do not exist at this wavelength. A more accurate *gf*-value for this line would therefore serve to better constrain the possibilities of an abundance enhancement versus unidentified features and be the first confirmed observation of a selenium line originating from a stellar photosphere.

A second example addresses the completeness of the UV atomic data available for synthetic spectrum analysis. Figure 2 presents a VUV ($\lambda < 2000$ Å) segment of the HST/GHRS spectrum of the chemically peculiar star χ Lupi A, a comparison of the observation with a synthetic spectrum computed by the author. It is clear that many features are not synthesized, either because the wavelengths or *gf*-values are not accurately enough known to include in the calculation or the features remain unidentified. For the VUV, the lack of atomic data can be partially attributed to a need for laboratory analyses. This is a result of limited resources (labs, researchers, funding) and to some extent a need for different optical material than that used at longer wavelengths. (Fourier-transform instruments for optical and (or) UV wavelengths typically use fused-silica optics, which absorb radiation for $\lambda <$ 1900 Å. The FTS at Imperial College London has a MgF_2 beamsplitter, allowing it to operate to wavelengths as low as 1400 Å.) Although atomic structure calculations have partially filled this data void, their accuracy can be highly uncertain if not constrained by experiment, as in the example in Fig. 1. For energy levels of high uncertainty and transitions having only one measured energy level, the wavelengths are not accurate enough to be included in synthetic spectrum calculations. This situation is well known to those computing synthetic spectra, who avoid using "predicted" wavelength data from the Kurucz database for "fine" analysis, but include them in opacity calculations.

A limitation to being able to test atomic data in the UV is the lack of wavelength-extensive observations of stellar spectral. UV atlases at high spectral resolution are few in number. Several bright star atlases exist from the Copernicus mission, but at a resolution that does not provide lines as narrow as their intrinsic linewidths for sharp-lined stars. The IUE satellite did cover long wavelength regions in a single observation (either 1200–2100 or 1900–3200 Å); however, the resolving power ($R = \lambda/\Delta\lambda = 11\,000$) resulted in strong line blending, which when coupled with the low signal-to-noise ratio (S/N typically 15) posed severe limitations on the study of weak features. Data quality was greatly improved with the HST instruments (GHRS, FOS, STIS, COS), although GHRS high-resolution observations had narrow wavelength intervals (~15 Å), and very few stars have extensive wavelength coverage obtained with this instrument. (For HST observing cycle 18, this situation will be remedied for cool stars if the ASTRAL Spectral Library observing program (PI T. Ayres) is successfully executed to record the complete spectra of eight cool stars with the STIS instrument.)

An intriguing target for atomic spectroscopy and stellar astrophysics is the bright star HD 72660 (HR 3383, A1 Vm), which was known to be iron rich from optical wavelength studies. The author has been analyzing this star for its post-iron-group element abundances, because it straddles the T_{eff} boundary near 10 000 K between the B type peculiar HgMn stars and hotter A type stars. An example of the need for conducting further atomic data studies at UV wavelengths is provided by the element tin. Figure 3 presents a 2 Å segment of the HST/STIS spectrum compared with the synthetic spectra generated by the author for the stellar parameters $T_{eff} =$ 9750 K, $\log g = 4.0$, solar-like metallicity with no atmospheric turbulence and a projected equatorial rotational velocity of 5.5 km s^{-1} [19]. The atomic line data were extracted from the database of Kurucz [20] (and updates since that time), which does not include line data for Sn II or Sn III. The calculated oscillator strengths of Oliver and Hibbert [18] were utilized for Sn II lines, including the 1811 Å line presented in the figure, as well as other identified Sn II lines in the spectrum of HR 3383 longward of 1600 Å. (The STIS spectrum of HR 3383 does not extend to wavelengths shorter than 1600 Å.) The tin abundance that best fits the data is an enhancement of 4.5 times the solar abundance. The figure also shows the location of a Sn III line, for which no oscillator strength exists, along with two strong unidentified iron lines.[4]

Tin is just one example of a post-iron-group element in need of atomic data. The UV spectra from Copernicus and IUE had foretold of a problem that HST would bring to bloom. The HST/GHRS observing program "The χ Lupi Pathfinder Project" (PI, D.S. Leckrone) rallied laboratory spectroscopists to provide accurate wavelengths, *f*-values, and line-structure parameters. Over a decade's work resulted in ultimately defining the abundance pattern for the heaviest stable elements, tantalum through bismuth [21, 22], and are

[4]S. Johansson. Private communication. 2006.

Fig. 2. The poor fit of synthetic spectrum (dashed) to the HST/STIS observation (solid) of χ Lupi is primarily due to missing lines in the calculation, either the result of unidentified features or unknown *gf*-value. Wavelengths of unidentified Fe lines, likely to be Fe II, measured in laboratory FTS spectra are provided along the top of the figure. (Figure and Fe line identification courtesy of Gillian Nave).

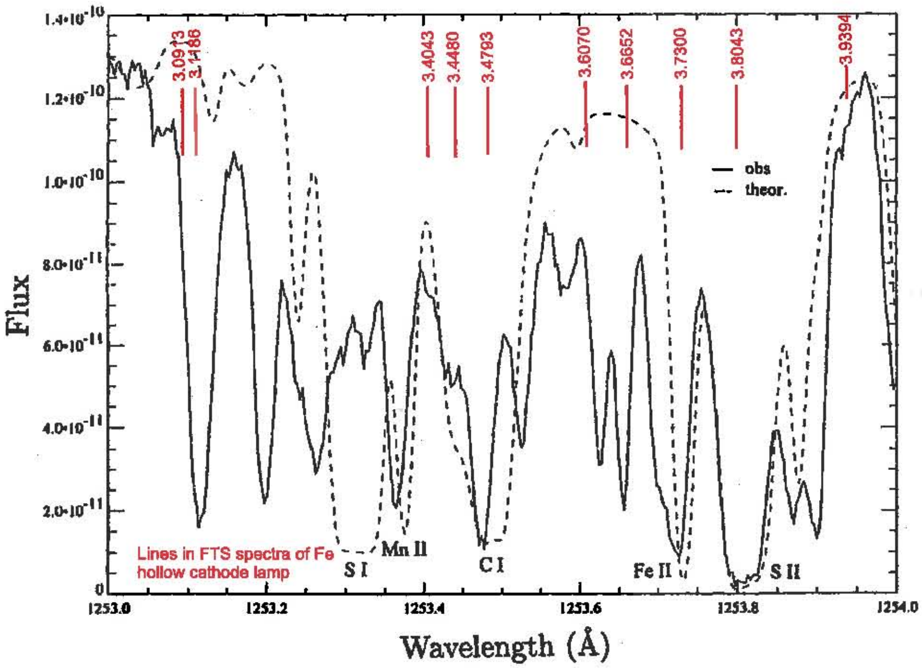


Fig. 3. The abundance of tin in HR 3383 (A1 Vm) is now determined, based on the calculations of *gf*-values for lines of Sn II [18]. In this small segment of the HST/STIS spectrum, compared with the synthetic spectra for the solar system value (dotted) and enhancement of a factor of 6 ([Sn/H] = +0.65 dex), the location of a Sn III line and unidentified Fe lines (Johansson, private communication) are noted.

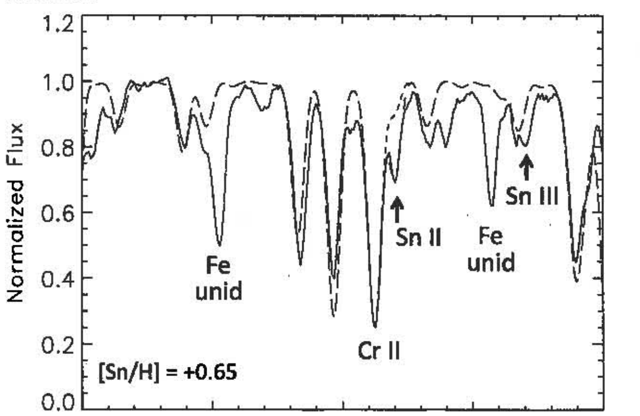
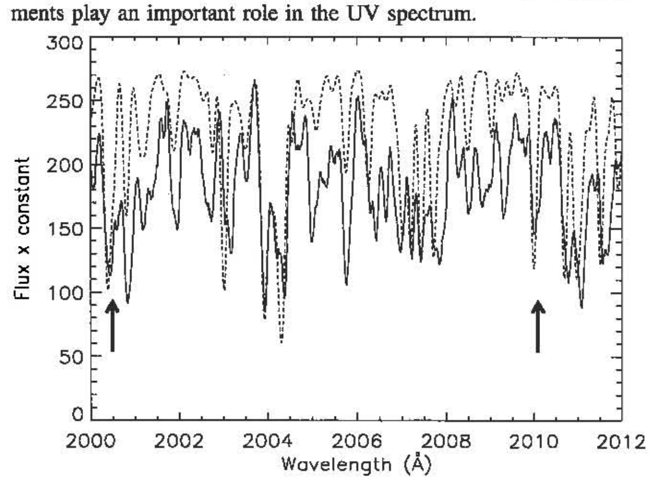


Fig. 4. The comparison of the HST/GHRS spectrum (solid) of the chemically peculiar star α^2 CVn with a synthetic spectrum (dotted) shows many features that are not properly fit. The locations of two Ce IV lines are noted, although they are not included in the calculation due to the lack of *gf*-values. For this hot star the rare-earth elements play an important role in the UV spectrum.



used for a broad array of stellar projects. Laboratory work related to this project continues to this day.

A final example of UV atomic data deficiencies are the spectra from doubly and triply ionized elements. The photospheric temperature of hot stars is sufficient to produce these spectral lines in absorption. Very few atomic data exist for these ionization states. Iron-group element data for the third spectra are critical to interpreting the spectrum at VUV and FUV wavelengths. Figure 4 presents a short segment of the GHRS spectrum of α^2 CVn (Bp) compared with a synthetic spectrum computed by the author for atmospheric conditions $T_{\rm eff} = 11\,500$ K, $\log g = 4.4$ to explicitly search for lines of CeIV, expected to be present from considerations of ionization potential and the presence of Ce III lines. This stellar spectrum shows strong enhancements of rare-earth element lines (REE, here meaning the lanthanides). Included in this calculation are all line data from the D.R.E.A.M. database [23]. The synthetic spectrum fit to the observation in

Fig. 5. A segment of the high-resolution NOT/SOFIN high S/N optical region spectrum of HR 3383 (solid) is compared with the synthetic spectrum (dotted). High-quality optical region spectra are able to be used to study weak lines of heavy elements, which might better be observed at UV wavelengths. Atomic data for optical transitions of iron-group and heavier elements need further attention.

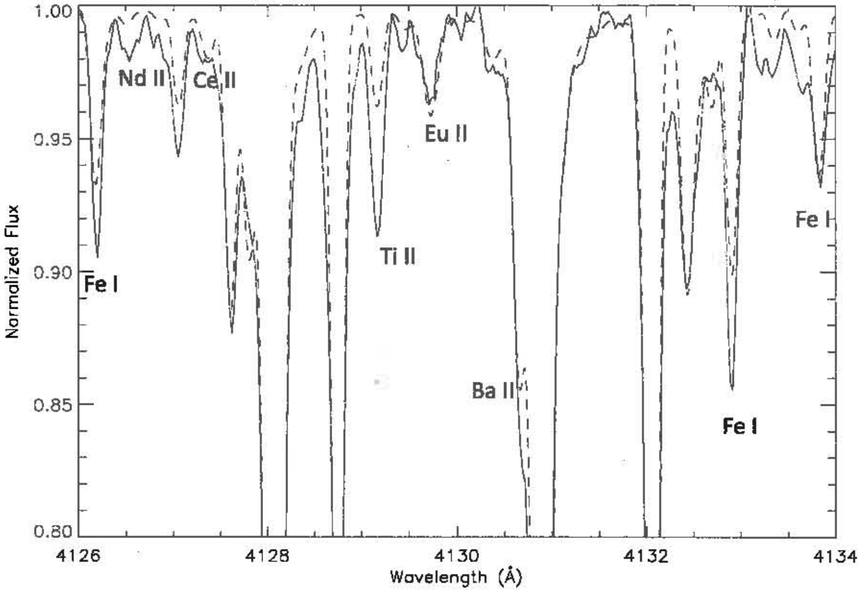


Fig. 4 is poor. The locations of the two strongest Ce IV lines (λλ2000.42, 2009.94 Å [24],) are noted, but they are not included in the calculation because of the lack of *gf*-values. The lifetimes of both upper levels ($5p^6$ $5d$ $^2D_{3/2,5/2}$) for these lines have been determined experimentally [25], but the BFs or calculated *gf*-values are not available. Although there are many unidentified lines, or improper element abundances, the search for Ce IV in this spectral region requires a better understanding of atomic spectra, in particular for the REE third and fourth spectra. Presently, no spectral line from the fourth spectrum of any lanthanide REE has been positively identified in a stellar spectrum.

4. The optical region: a work in progress

The optical region is home to low-excitation lines of most elements. Although it is dominated by lines from iron-group elements, heavier elements are well represented. The wavelength limits of the optical region have been defined by earlier astronomical detectors and human vision, as a region spanning from Ca II H and K to Hα, roughly 400 to 700 nm. As a result of improvements in detector technology, this region has been expanded to approximately 300 to 1100 nm. The expanded wavelength coverage has increased the efficiency of recording spectra, which for some stars can be bracketed by the light elements Be II λ313.1 nm and He I λ1083.0 nm, both of which are the only viable lines, for their respective elements in the optical region, for analysis in cool star spectra.

Expanding the optical domain also increases the demand on atomic data. However, considering that laboratory instrumentation has typically included the near-UV and red spectral regions, there is little extra burden placed on laboratory spectroscopy. On the contrary, its capabilities are now being more fully utilized by astronomers.

The relatively recent opening of the near-UV and near-IR spectral regions for high-resolution astronomical spectroscopy will be dramatically offset by the closure of the UV (120–320 nm) when the HST instruments are no longer functioning. With no plans for follow-up capabilities for UV spectroscopy, a tremendous blow will be dealt to stellar astrophysics. It is equally deleterious to other branches of astronomy, but perhaps most problematic to interstellar medium studies, which rely on the UV for the many resonance lines of singly-ionized species that are located in that region. The potential of the World Space Observatory (WSO, wso.inasan.ru) will be eagerly followed to fill this void. Although interest exists for UV spectroscopy, its absence in the recently released Decadal survey [26] will likely exclude it from serious consideration by US funding sources for near-term missions.

With the impending loss of UV spectroscopy from space, even if for a brief period of time, UV spectral diagnostics will need to be replaced by diagnostics at optical and IR wavelengths. This is currently within present-day instrument capabilities but requires the cooperation of both astronomers and atomic data producers. Figure 5 presents an 8 Å segment of the spectrum of HR 3383, obtained with the SOFIN echelle spectrograph [27] on the 2.6 m Nordic Optical Telescope (NOT). The high-resolution ($R = 80\,000$) observation is compared with a synthetic spectrum created by the author, using the ATLAS/SYNTHE suite of programs [28]. The abundances for iron-group elements were determined from spectral lines having laboratory determined *f*-values, which are not present in the figure.[5] The comparison clearly depicts iron-group element lines (Fe I, Ti II) having *f*-values discordant from those used for the abundance determinations. Also obvious in the figure is the presence of weak features from post-iron-group elements (Nd, Ce, Eu, Ba) as well as features not properly synthesized, perhaps a result of uniden-

[5]Wahlgren et al. Manuscript in preparation.

tified or unclassified lines or poor f-values. Although weak iron-group lines might be neglected in favor of stronger unsaturated lines for abundance analysis, the utility of weak lines for atmosphere analysis should not be neglected, since a range of line strengths is needed to probe the depth of the photosphere. The weakest features, within 1%–2% of the continuum, are made useful by the rather high S/N (~150 in the continuum). To exploit weak spectral features, stellar spectra must be obtained at high resolution and high S/N, preferably at levels of $R = 10^5$ and S/N > 300, respectively. For bright stars, modern detectors can record spectra in a short amount of time. The advantages are many if the atomic data exist to interpret the stellar spectra. Data producers must work to include weak lines in their analysis and reduce the uncertainty in the f-values of weak lines.

In addition to extending knowledge to include weak lines, the general problem of data for lines at higher excitation energies also exists. These two problems are not mutually exclusive. Weak emission lines (WELs) have been catalogued at optical wavelengths in spectra of hot stars (see [29] for a review on WELs and [30] for a catalogue of WELS in the spectrum of 3 Cen A). Lines from iron-group and lighter elements are observed at a level of several percent of the continuum and originate from high-excitation levels (for Fe II, $E_{low} > 60\,000$ cm^{-1}). Most of the WELs do not have oscillator strengths. The observed emission line intensities have been correlated with element abundance and will be an important constraint for the study of diffusion and chemical peculiarity in hot stars. But to do so requires accurate oscillator strengths for lines at high-excitation energies for those elements identified to produce WELs.

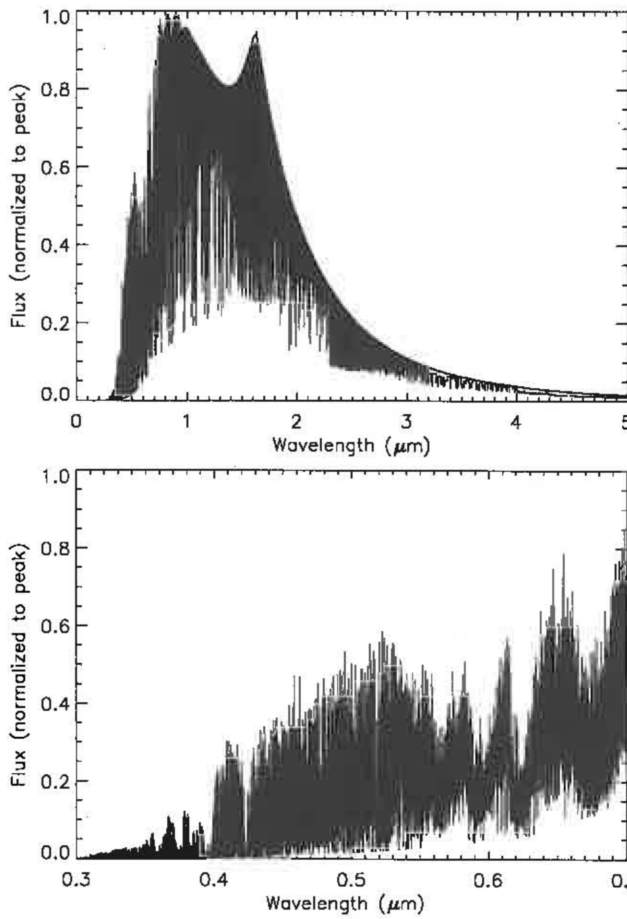
High excitation lines of low charge states are also important as absorption features in stellar spectra. The iron-rich, hot star HR 6000 (Bp) has been the subject of study at optical wavelengths for the purpose of identifying many strong features that have been shown to be high excitation lines from Fe II. Johansson [3] used this spectrum to identify lines from the 4d–4f transitions previously not detected in laboratory spectra. These same stellar data were used to identify 50 new energy levels and the lines associated with them [10, 31]. Additional levels and lines in Fe II, and other single-ions from the iron group, are no doubt waiting to be discovered at optical and IR wavelengths.

5. A renaissance for the IR

The history of astronomical IR spectroscopy for quantitative analysis dates back to the 1960s and 1970s when low- to moderate-resolution spectra at regions from 1 to 10 μm showed the strong presence of molecular bands in cool star spectra and were profoundly important for measuring isotopic compositions of light elements in molecules such as CO and H_2O (cf., [32–35]). The IR remained the domain of cool star research but would not provide a better understanding of chemical abundances, for instance, than what could be obtained at optical wavelengths with higher spectral resolution. The applications of low-resolution IR stellar spectroscopy have been expanded to include spectral classification [36, 37] and population studies in galaxies.

The IR is an extensive region. Modern instrumentation has lead to a working division of the IR into subregions: the

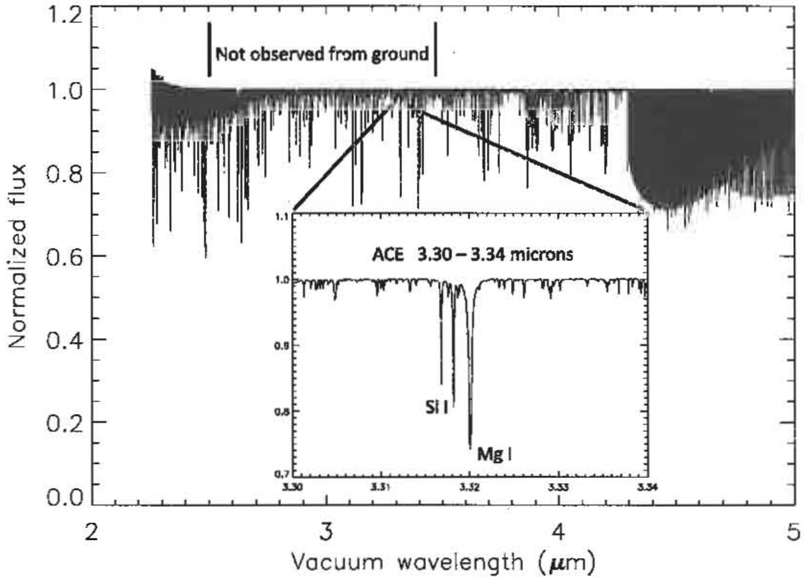
Fig. 6. The spectral energy distribution for a cool giant star (M3 III, $T_{eff} = 3500$ K, $\log g = +1.0$), taken from the MARCS stellar atmosphere code on-line distribution, shows the majority of stellar flux to be radiation at near-IR wavelengths. (*upper panel*) The smooth nature of the near-IR spectrum implies the presence of a detectable continuum level. (*lower panel*) The continuum level is not observed at optical wavelengths because of the strong absorption from the molecules TiO and CN, making detection and analysis of atomic lines difficult.



near-IR (1–5 μm and an earlier association with the 0.7–1.0 μm region), the mid-IR (5–40 μm) and the far-IR, before reaching the sub-millimetre region. For the study of stellar photospheres, 5 μm is a useful upper limit designation. At longer wavelengths, the circumstellar environment, in the form of a disk or warm dust for both pre-main-sequence and main-sequence stars, is likely to contribute to the observed spectrum. In addition, the stellar flux is reduced and atomic lines originating from the photosphere are few. The 5–10 μm region might be considered a transition region for stellar astrophysics.

The IR is important to stellar astrophysics. Cool stars have a majority of their flux near or beyond 1 μm. Figure 6 presents an SED computed for a cool giant star ($T_{eff} = 3500$ K, $\log g = 1.0$) of solar metallicity (i.e., oxygen-rich, as opposed to carbon-rich chemistry). At optical wavelengths, strong blanketing of the flux from molecules (CN, TiO in particular) renders delineation of the continuum nearly im-

Fig. 7. A segment of the high-resolution spectrum of the sun from the Advanced Chemistry Experiment (ACE) satellite, which fully extends from 2.3 to 14 μm, is displayed. The insert presents several strong atomic absorption lines not observed from the Earth's surface.



possible, along with the study of weak lines. Element abundances for cool stars ($T_{\rm eff} < 3800$ K) have not been determined for elements that do not produce strong lines at optical wavelengths. At near-IR wavelengths, the computed SED is seen to be smooth, implying the continuum level can be identified through the molecular bands of OH (1.6 μm), CO (1.6, 2.3, 4.05 μm), and SiO (4 μm).

The IR is also important for studies of magnetic field strength (a property that is proportional to λ^2), accurate radial velocity measurements, and the presence of certain molecular (CO, SiO, among others) and atomic (C, N) species not observed at optical wavelengths. The characterization of exoplanet atmospheres is currently conducted at mid-IR (5–10 μm) wavelengths [38].

However, exploiting the IR does not come without difficulty. Special consideration must be given to detectors and telescope design (the latter to avoid thermal radiation), observing sites with the proper weather conditions (low water vapor), proper modeling of the terrestrial atmospheric spectrum, limitations imposed on the photospheric SED by circumstellar material (typically in the early and late stages of stellar evolution), and atomic and molecular line data are desperately needed for line identification and quantitative analysis.

The paucity of wavelength and oscillator strength data at IR wavelengths can be regarded as a consequence of astronomical need. At the lower spectral resolution offered by earlier instrumentation, line blending limited the identifications to the strongest features. The exceptions are the sun, which had been observed at high spectral resolution by instruments at KPNO, the space experiments ATMOS and ACE (Atmospheric Chemistry Experiment [39]), the cool star Arcturus (K2 Ib) [40], and a limited number of KPNO 4m FTS observations of stars in the K band [41]. Line identifications have been provided by [42–45] for elements no heavier than the iron group. Figure 7 displays the ACE spectrum for wavelengths shorter than 5 μm, with an insert showing several lines not visible from ground-based observatories. This impressive spectrum extends into the mid-IR region (2.3–14 μm) and can serve a variety of purposes, both for astronomy and general spectroscopy.

Very few laboratory oscillator strengths, 118 in total are listed in the NIST on-line database, exist for transitions at wavelengths longer than 1 μm. These have been primarily limited to iron-group elements. Comprehensive calculations of *f*-values from the UV to the IR have been provided by R. Kurucz for many neutral elements and several single ions. Limited laboratory *gf*-values for other elements are available (for example, Mn I [46] and Sm II [47]).

Astrophysical *gf*-values for lines in the J and K photometric bands are also available, based on the solar spectrum [48, 49]. For the 847–874 nm region, the region to be observed at moderate resolution ($R \sim 11\,500$) by the ESA/Gaia radial velocity spectrometer, data have been provided by [50], but additional atomic data are required.

The problem with IR atomic data is twofold:

- Modern laboratory spectra are lacking for most — essentially all — elements for wavelengths longer than 1 μm. These data are required for line identification.
- Oscillator strengths are needed. The data that are most deficient are branching fractions (BF_{ji}), which are used with the level lifetime τ_j to determine transition probabilities A_{ji}, via the relation,

$$A_{ji} = \frac{\mathrm{BF}_{ji}}{\tau_j} \tag{4}$$

which are then transformed into oscillator strengths via the analytic expression,

$$f_{ji} = 1.499 \times 10^{-8} \frac{g_j}{g_i} \lambda^2 A_{ji} \tag{5}$$

where A is in units of 10^8 s^{-1} and λ is in Å.

The accuracy of the *f*-value is dependent on the accuracy

Table 1. The number of rare-earth element transitions are presented for the UV (120–310 nm), optical (310–1000 nm), and IR (1000–5300 nm) wavelength regions for neutral (I), singly-ionized (II), and doubly-ionized (III) states, along with the number of energy levels (*L*) associated with these transitions (italics).

ID	L I	UV I	O I	IR I	L II	UV II	O II	IR II	L III	UV III	O III	IR III
La	*304*	152	5451	5393	*121*	585	960	279	*41*	60	63	49
Ce	*982*	0	4336	33940	*500*	3148	14563	6435	*221*	1784	1725	733
Pr	*412*	0	5824	10809	*208*	0	2801	1443	*400*	8157	4295	1049
Nd	*709*	0	12000	22553	*829*	695	18174	14394	*28*	0	55	0
Sm	*471*	22	6129	3048	*376*	112	7552	954	*42*	44	58	0
Eu	*123*	20	831	674	*170*	396	2380	730	*143*	1083	494	90
Gd	*612*	543	15773	16473	*314*	488	5899	3478	*25*	56	2	28
Tb	*590*	32	12905	4217	*152*	158	1711	1555	*111*	947	265	83
Dy	*719*	181	21671	26768	*562*	930	18092	7547	*106*	1156	244	1
Ho	*234*	42	2720	3615	*100*	53	591	208	*121*	1047	470	57
Er	*670*	272	16133	18982	*360*	777	6329	2378	*115*	1025	446	4
Tm	*508*	182	9300	13189	*361*	2190	11071	1163	*120*	1072	578	11
Yb	*224*	87	1659	3023	*337*	2716	8098	2284	*66*	296	83	31
Lu	*187*	223	1687	1500	*41*	71	165	26	*28*	32	35	7

of λ, τ, and BF (through the line intensity). Although measurements of IR spectral line intensities can be highly accurate, for weak lines originating from the same upper level as strong UV and (or) optical transitions, the main difficulty lies in analyzing the uncertainty in the BF.

Existing laboratory analyses at optical and UV wavelengths provide accurate energy levels that can be used to determine IR wavelengths by the Ritz combination principle. Additionally, atomic lifetimes and HFS constants are also available for levels associated with some near-IR lines. However, there are many unidentified features in stellar near-IR spectra. New laboratory spectra may identify spectral lines, whose energy levels would only be determined from IR lines. The discovery potential for new energy levels from laboratory IR spectroscopy is high.

An important consideration when planning new laboratory projects in near-IR spectroscopy is knowing the extent to which transitions may be important for stellar studies. We consider the number of spectral transitions in different wavelength regimes for the lanthanide REEs, based on known energy levels of neutral, singly-ionized, and doubly-ionized species. (The lanthanides continue to be of interest to astronomy. The reasons for this include their large number of transitions from the UV to the IR, line-structure broadening due to HFS, IS, and magnetic effects, and their utility as diagnostics for neutron-capture nucleosynthesis — the r- and s-processes.) Energy levels were taken from the compilation of Martin [51], complemented by publications since that time for the spectra Ce III [52], Ho II [53], Dy III [54], Eu III [55], Er III [56], and Yb III [57]. Table 1 provides the number of levels included in the calculations and the number of transitions for the UV (120–310 nm), optical (310–1000 nm), and near-IR (1000–5300 nm) spectral regions. The number of allowed transitions was determined by accounting for the quantum mechanical selection rules for parity and total angular momentum *J*. The results are to some extent intuitive. Neutral elements have few transitions in the UV relative to the IR, while the opposite is the case for the third spectra. Neutral-species transitions do not exist for wavelengths shorter than about 200 nm, due to the low first-ionization potential of the REEs. (The tabulated numbers are a guide to the distribution of transitions by astronomical spectral region, as defined by certain instrumentation. Transitions are not equally distributed in wavelength. Shifting the boundaries by as little as 100 nm may have a large effect on the perceived distribution.)

Table 1 does not address the number of transitions that may be detectable and (or) useful in stellar spectrum analysis. Through collisions, the population of energy levels in a stellar photosphere is a function of temperature (and to a lesser extent stellar luminosity or pressure). The temperature structure of the atmosphere will dictate the proportion of an element in molecular versus atomic or ionic state with atmospheric depth, the population of energy levels, and indirectly, opacity (line density). The observed line depth or another measure of line intensity, such as the equivalent width, will depend on the element abundance in the line formation region. By way of example, it would be expected to identify Eu II lines in the near-IR spectrum of the magnetic chemically peculiar star HD 118022, most obviously because strong lines of Eu II are present in its optical spectrum. But of the 810 transitions identified in Table 1, we might only expect to identify 16 lines, those with lower energy level near 16 000 cm^{-1}. All other Eu II lines have a lower level near 50 000 cm^{-1}, which when coupled with relatively low *gf*-values, will not produce a detectable spectral line. Figure 8 shows the Eu II λ1002 nm line as a weak feature. The high-excitation lines will be orders of magnitude fainter. For cooler stars, the population of energy levels near 20 000 cm^{-1} is further reduced, and we will expect to find only low-excitation lines of Eu I or Eu II.

As a general statement, it can be said that not all stars require the same atomic data, and not all spectral transitions will be observable. As a caveat, lower excitation lines require our first attention.

Although the current discussion of atomic data for the IR has thus far been restricted to the near-IR, long-standing data needs and new developments in instrumentation for the mid-IR provide opportunities for atomic data studies for applications in stellar astrophysics. The satellite observatories Infrared Space Observatory [59], AKARI [60], and the Spitzer Space Observatory [61] have produced a wealth of low-reso-

Fig. 8. The presence of Eu II λ1002 nm is noted from the spectrum comparison of e Vel (HD 73634, A6 II) with the chemically peculiar star HD 118022 (A2p) and a synthetic spectrum calculation made for the atmospheric conditions $T_{eff} = 9000$ K, $\log g = 4.0$ and an enhancement of europium by a factor of 10 over the solar system value. The fixed-pattern noise seen in these ESO/VLT UVES (UV–visual echelle spectrograph) spectra is not present in the ESO/VLT CRIRES (cryogenic high-resolution IR echelle spectrograph) spectrum. A CRIRES observation of HD 118022 will be made in the future [58].

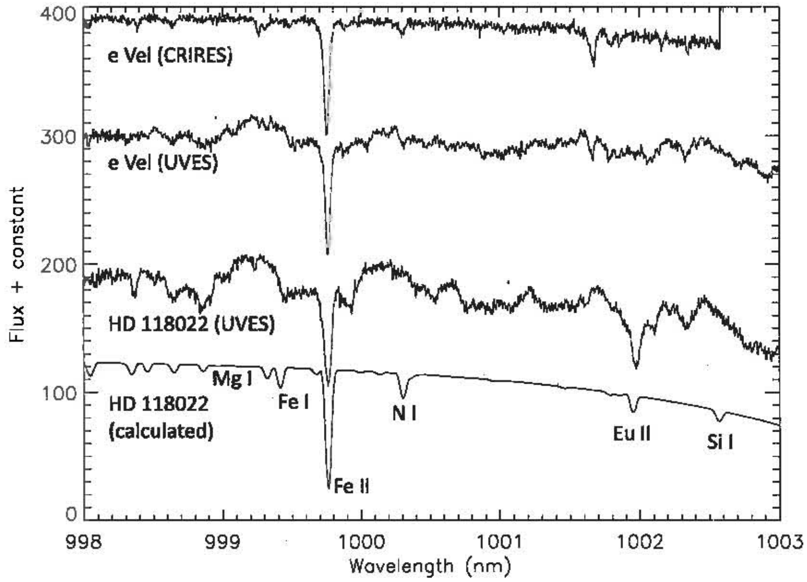
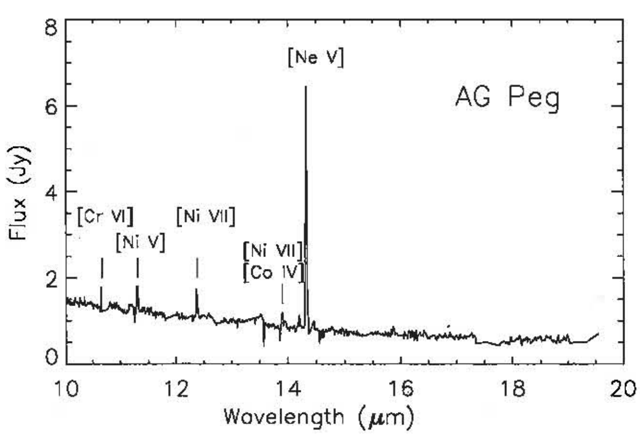


Fig. 9. Fine structure lines in the Spitzer Space Telescope spectrum of the symbiotic star AG Peg.



lution spectra ($R < 1000$). In this realm of fine-structure lines, many emission lines remain unidentified. Figure 9 presents part of the Spitzer spectrum of the symbiotic star system AG Peg. (Symbiotic stars are binary star systems comprised of a red giant and a white dwarf in relatively close proximity, such that the high-energy photons from the white dwarf ionize and excite material in the cool star wind, resulting in a high-excitation emission line spectrum and cool star photospheric spectrum — a symbiotic spectrum.) Several fine-structure emission lines are labeled. Other features, which may be real, remain unidentified. The sensitivity of the Spitzer detectors will be improved upon by future instruments, e.g., those planned for the Stratospheric Observatory for Infrared Astronomy (SOFIA) airplane observatory and the James Webb Space Telescope (JWST). New ground-based instrumentation is now available for the mid-IR, such as the ESO/VLT/VISIR spectrograph, which is capable of taking spectra in the photometric N (8–13 μm) and Q (16.5–24.5 μm) bands with resolving powers in the range $R =$ 150–30 000. Improvements in detector sensitivity will reveal new features that will require atomic data for identification and analysis. The importance of accurate and complete compilations of atomic lines for both identification and analysis lies in the ability to model the emission line spectrum for gas temperature and element abundance. In an optically-thin plasma, the element abundance of a given species must be determined from multiple ions.

The identification of fine-structure lines has been undertaken using spectra [62, 63] from the Infrared Space Observatory (ISO) SWS instrument. Ritz wavelengths have also been determined for parity forbidden transitions in [Cr II], [Ti II], and [Fe II] from experimentally determined energy levels involving the lowest even parity LS terms [64]. Compilations of fine-structure lines include the NIST atomic spectra database, which for example, lists 121 lines in the region 5–40 μm having $E_{low} < 5000$ cm^{-1} and the Atomic Line List [65]. The accuracy and completeness of fine-structure line wavelengths requires further attention.

6. Summary

The need for atomic line data for the analysis of stellar spectra is greater now than it ever has been. From the UV to the IR, spectral data is used to determine stellar atmospheric parameters and investigate formation processes and interactions of stars with their environment. In the past decade, atomic data for UV and optical wavelengths has been a prominent part of long-term studies of the sun, chemically peculiar stars, metal-poor stars, and the luminous star η Carina. It should also be mentioned that individual spectroscopists and theoreticians have taken a personal interest in these projects and have therefore played a key role in supplying the necessary data. These undertakings will continue to benefit from improved atomic data. New endeavors that require a large amount of atomic data, such as neutron star mergers to produce the r-process elements during gamma-ray bursts [66], will capture our imagination.[6]

Stellar astrophysics in the UV remains a vibrant research arena, where there is a continuing need for new atomic data, especially below 2000 Å. We have still not acquired an adequate understanding of the UV spectrum for many elements. Now, on the verge of an IR explosion in applications for extragalactic astronomy, the failings of the UV become redshifted into the optical and infrared. But whether the spectra are from stars in the neighborhood observable at UV wavelengths at high spectral resolution or distant sources observed at low resolution in the optical or IR, a common priority for atomic data remains the iron-group elements. The Fe II spectrum is ubiquitous and needs to be better understood to define its role in line blending and opacity at all (rest) wavelengths. Another priority continues to be oscillator strengths for ground-state resonance transitions for low charge states, since these are important to both studies of the interstellar medium and hot star photospheres.

The demise of UV spectroscopy from space reflects a shift of priorities for major space projects in the near future. The optical spectral region can be further worked to develop diagnostics to complement those in the UV. In particular, weak lines of post iron-group elements and high-excitation lines from low charge states offer opportunity for spectroscopic analyses.

New instrumentation for current and planned ground-based and space observatories for IR spectroscopy are placing ever higher demands on atomic data. Recent and ongoing research provides a rich selection of topics for stellar astrophysics in the near-IR, such as magnetic fields in post main-sequence stars, circumstellar disks, metallicity studies for stars with exoplanets, characterizing the atmospheres of exoplanets, and light element analysis for stellar population studies. For the near-IR wavelength region (1–5 μm), accurate wavelengths are needed to enable line identification at high spectral resolution. Few transitions have laboratory determined oscillator strengths for the near-IR, and in particular the lines from iron-group elements are important for metallicity studies and line blending, while post iron-group element data are needed for investigating nucleosynthesis via the r- and s-processes in evolved stars. For mid-IR wavelengths, a particularly useful undertaking will be to expand our knowledge of atomic line data for ground-state fine-structure lines, as these are seen in a variety of emission line targets (planetary nebulae, symbiotic stars, and active galaxies and quasars).

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