In search of the $s$-process in cool supergiants: 
A vital role for laboratory astrophysics

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Abstract. We report on progress in determining the chemical composition of the photospheres of massive, cool supergiant stars for the purpose of investigating whether by-products from recent slow neutron capture nucleosynthesis have been transported up to the photosphere by convective processes. Our initial work has been focused on identifying atomic transitions that are useful for stellar abundance work at near-infrared wavelengths and in gathering accurate atomic data for these transitions. The latter task includes the determination of experimental oscillator strengths, which represents a vital role for laboratory astrophysics. We use high-resolution optical and near-infrared spectra of the massive, cool star $\alpha$ Orionis as the prototype for our study for line identification and synthetic spectrum modeling. Abundances have been determined for a number of heavy elements, and our early results illuminate the problems with atomic data that must be overcome before we are able to derive chemical abundances with the accuracy required for meaningful comparison with calculations for $s$-process nucleosynthesis.

1. Introduction
The creation of isotopes for elements heavier than the iron group is primarily attributed to the capture of free neutrons by pre-existing nuclei. Two main groupings of neutron capture processes are known, defined by the rate at which neutrons are captured. The capture rate can be compared to the rate at which unstable nuclei decay via transmutation of a bound neutron into a proton and electron, known as $\beta$ decay. Neutron capture in explosive events, such as novae and supernovae, occurs more quickly than $\beta$ decay, and is referred to as rapid neutron capture ($r$-process). The $r$-process is capable of creating isotopes for essentially all elements heavier than zinc, including the actinides. When neutron capture rates occur on time scales that are similar to $\beta$-decay rates, the process is referred to as slow neutron capture ($s$-process).

The $s$-process is theorized to occur at different sites, with the main $s$-process occurring in the interiors of low-mass red-giant stars and asymptotic giant-branch stars, while the weak $s$-process, attributed to a lower neutron exposure, occurs in massive supergiants during the phases of core helium burning and shell carbon burning. Calculations ([1], [2]) utilizing large nuclear-reaction networks show that $s$-process efficiency increases with stellar mass in the mass range 15 to 30 solar masses, and abundance enhancements for $s$-process nucleosynthesis are highest for
certain isotopes of post iron-group elements, in particular, germanium, selenium, krypton, and strontium. For cool supergiants, the detection of individual isotopes can only be realized through spectrum analysis of molecules. However, if these isotopes contribute a dominant fraction of the element’s total abundance prior to the initiation of the $s$-process, then a resulting increase in their abundance by factors of 10 to 100 will lead to an observable effect in the spectrum, provided that the enriched material can be transported upwards into the photosphere. Freytag et al. [3] have performed 3D stellar convection modeling for the supergiant $\alpha$ Orionis (spectral type M2 Iab), showing that convection can reach significant depths into the stellar interior. Therefore, the ability to determine chemical abundances will lead to an improved understanding about both $s$-process nucleosynthesis in stellar interiors and convective processes.

Studies during the 1970s and 1980s ([4], [5], [6], [7], [8], [9]) determined chemical abundances from optical region spectra for G and K type supergiants. For these low-mass supergiants no abundance enhancements were observed that could be explained by dredge-up of $s$-process material. Among low-mass giant stars of spectral types MS and S it is well known that lines of $s$-process elements are enhanced in the spectrum (see for example [10]). More recent elemental abundance studies of cool giants and supergiants make use of the near-infrared (near-IR) spectral region, but limit the analysis to carbon, nitrogen, and oxygen in molecular species and the strongest atomic lines of aluminum, magnesium, silicon, calcium, titanium, and iron (see for example [11], [12]) due to unknown oscillator strengths for other species. The determination of heavy element abundances for cool, massive supergiants has been very limited. Vieira [13] analysed a segment of the IR spectrum (1.1 to 1.35 $\mu$m) of $\alpha$ Orionis for elements no heavier than zinc.

For cool stars (type M), the near-IR spectral region (for our purposes taken to be from 0.8 $\mu$m to 5 $\mu$m) offers the benefits of higher stellar flux and a reduction in molecular absorption from the stellar atmosphere over use of optical wavelengths. For ground-based observations, the usable wavelengths are limited to windows of the Earth’s atmosphere, while for space or airborne observatories these windows expand to include all wavelengths, which more than doubles the effective wavelength coverage for near-IR observations.

We have initiated an investigation of cool, massive supergiants, where our goals are to: 1) identify spectral lines at near-IR wavelengths, in particular for elements heavier than the iron group; 2) determine accurate atomic data for these lines, if necessary through new laboratory measurements; and 3) determine abundances for the elements relevant to the weak $s$-process ($Z = 30$ to 42). The stellar abundances will be interpreted in terms of nucleosynthesis models to ascertain whether the by-products of the weak $s$-process have been dredged up to the photosphere by convective processes. In this contribution we present our methodology and early results, concentrating on the subject of atomic data for elemental abundance analysis of the massive supergiant $\alpha$ Orionis.

2. Analysing the spectrum of $\alpha$ Orionis

We begin our investigation of chemical abundances in cool, massive supergiants with $\alpha$ Orionis, which is the prototype for this study as a result of its sharp-lined spectrum and availability of high-resolution spectra. Although its mass is not accurately known, $\alpha$ Orionis is considered to be massive (15 to 25 solar masses) by virtue of its luminosity and spectral features. Our analysis makes use of high spectral resolution data obtained with the 2.5 m Nordic Optical Telescope Soviet-Finnish echelle spectrograph and archival data from the Kitt Peak National Observatory (KPNO) 4 m IR Fourier transform spectrometer (FTS) [14] and the European Southern Observatory (ESO) Very Large Telescope (VLT) Ultraviolet and Visual Echelle Spectrograph (UVES).

An additional consideration to derive accurate abundances is the construction of an appropriate model atmosphere for an extended atmosphere such as that of $\alpha$ Orionis. The
location of formation for a spectral line within an atmosphere will depend on characteristics of the energy levels (energy, lifetime) and the environment (temperature, density) in which the atoms are immersed. A spectral line will have contributions to its profile from a range of atmospheric conditions, which may exacerbate the choice of model atmosphere codes based on local thermodynamic equilibrium (LTE) or non-LTE conditions or, similarly, between plane-parallel versus spherical geometry. Our use of plane-parallel, LTE model atmospheres is satisfactory for our work in identifying spectral lines, gauging uncertainties, and estimating abundances for comparison with theory for many spectral lines. For lines formed under conditions of non-LTE, we will synthesize the spectrum using non-LTE codes to provide a more accurate abundance.

The LTE model atmosphere was generated using the ATLAS12 code [15]. The atmosphere parameters ($T_{\text{eff}} = 3550$ K, gravity log $g = -0.2$, microturbulent velocity = 3.1 km s$^{-1}$, macroturbulent velocity = 11 km s$^{-1}$) were determined by fitting near-IR spectral features that are sensitive to temperature and luminosity (CO 2-0, 3-1 bandheads; Fe I lines; CN lines). Although this characterization of the model is used for all of our spectra, we are mindful that $\alpha$ Orionis is known to show weak photometric and spectrum variability, and that the optical and near-IR spectra we analyze were taken years apart.

To date, abundances for 23 elements have been derived ([16], [17]) by fitting the observed data with spectra generated with the SYNTHE code [18], which includes molecules for both the equilibrium calculations and the line spectrum. Although the uncertainties are large, the elements cobalt, nickel, copper, rubidium, yttrium and zirconium have similar abundances in $\alpha$ Orionis to those in our solar-system. However, the abundances of germanium and strontium are 2.1 times higher (+0.33 dex) and 25 times higher (+1.4 dex), respectively. If the enhancements are confirmed by further analysis, taking into consideration new atomic data and non-LTE calculations (for Sr II lines), then they may provide evidence that the s-process is operating at interior layers and that its by-products are being dredged-up to the photosphere. Such a result may be commensurate with our knowledge of the carbon isotope ratio, $^{12}$C/$^{13}$C < 20, for $\alpha$ Orionis ([19], [20]), if there exists free neutrons produced by the $^{13}$C($\alpha$,n)$^{16}$O reaction. We have not yet investigated abundances for other elements relevant to the weak s-process due to limited wavelength coverage of the stellar observations and the lack of atomic data.

3. Atomic data for the IR

The chemical abundances that we have determined for $\alpha$ Orionis are assigned uncertainties that are too large for a meaningful comparison to be made with nucleosynthesis calculations. The uncertainties are as large as a factor of 4, and are the result of line blending, uncertain atomic data and, to some extent, the approach employed to calculate model atmospheres and synthetic spectra for supergiant stars. For the vast majority of near-IR transitions, $g$-f-values have been calculated by R. Kurucz, and have an unknown accuracy. Few transitions of elements heavier than the iron group have $g$-f-values for wavelengths longer than 1 $\mu$m.

Oscillator strengths determined from fitting line profiles or equivalent widths in stellar spectra, assuming an abundance for the element and a model stellar atmosphere, are commonly referred to as astrophysical $g$-f-values and are available for some near-IR transitions based on analysis of the solar spectrum [21]. However, astrophysical $g$-f-values should be used with caution since they could be enhanced or made deficient by underestimating or overestimating, respectively, the absorption associated with line blending, as well as bound-free and free-free sources of opacity. For cool stars, including the Sun, the treatment of molecular absorption is of particular concern at IR wavelengths when determining astrophysical $g$-f-values or abundances from spectral line analysis. Uncertainties in the parameters (effective temperature, gravity, chemical composition) used in generating the atmospheric model with which astrophysical $g$-f-values are derived will impart additional uncertainty to the $g$-f-values.
The six stable isotopes of selenium are present in the light source in their terrestrial mixture but do not result in observable isotope or hyperfine structure.

Large uncertainties in atomic and molecular data also lead to misinterpretation of line blending and continuum placement. For cool, oxygen-rich stars (i.e., oxygen to carbon abundance ratio greater than unity) such as α Orionis, the problem of continuum placement at near-IR wavelengths is more tractable than at optical wavelengths due to the nature of the molecular absorption. The prominent contributor to absorption at optical wavelengths is TiO, with contributions from CH and CN at blue wavelengths, while at near-IR wavelengths many weak lines from CN are evident.

3.1. Atomic data for Se\textsc{i}

Selenium is an important element for the study of the s-process in massive supergiants. In addition, lines from Se\textsc{i} and Se\textsc{ii} have never been identified or analyzed in stellar spectra, including that of the Sun, in part as a result of insufficient atomic data. We have initiated laboratory spectroscopy of selenium that will lead to improved atomic data for spectral lines in Se\textsc{i} and Se\textsc{ii}. The selenium spectrum for the wavelength interval from 400 nm to 1100 nm was recorded using the 2 m FTS at the National Institute of Standards and Technology. The light source was a hollow cathode lamp with selenium pellets placed inside an aluminum cathode. Argon, neon, and a helium-neon mixture were used as carrier gases. Figure 1 displays a segment of the new laboratory data, showing the Se\textsc{i} transition 5s $^5S_2$ - 5p $^5P_2$. The three multiplet transitions present strong lines in our laboratory data and their lower energy level (48 182.2 cm$^{-1}$) is weakly populated in the photospheres of cool stars.

Additional laboratory spectra of selenium will be obtained for wavelengths below 400 nm and above 1100 nm, which will allow us to measure accurate wavelengths and line intensities, determine accurate branching fractions, and possibly revise and extend the energy level systems of Se\textsc{i} and Se\textsc{ii}. The branching fractions will be combined with atomic lifetimes to determine oscillator strengths.
4. Summary
From our analysis of the $\alpha$ Orionis spectrum two statements regarding atomic data can be made:

- At near-IR wavelengths there are many atomic lines of heavy elements which would be useful for abundance analyses if accurate atomic data existed.
- Improvements to currently available $gf$-values will allow tighter constraints to be placed upon the derived abundances for $s$-process elements, which will enable meaningful comparisons of abundances with the nucleosynthesis calculations.

Stellar spectrum analysis in the near-IR is currently hindered by the atomic data and will require the efforts of both laboratory spectroscopists and theoreticians to produce accurate and complete data sets for neutral and singly-ionized species for the study of cool stars.

Our investigation of the $s$-process in massive stars will continue with new and archived stellar spectra of luminous stars at near-IR wavelengths, creating new laboratory atomic data for $s$-process elements, and investigating the influence of non-LTE physics and spherical model atmospheres on the determination of elemental abundances.

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References
[1] The L-S, El Eid M F and Meyer B S 2000 ApJ 533 998
[2] The L-S, El Eid M F and Meyer B S 2007 ApJ 655 1058
[3] Freytag B, Steffen M and Dorch B 2002 AN 323 213
[4] Bakos G A 1971 JRA SC 65 222
[5] van Paradijs J 1973 A&A 23 369
[6] Luck R E 1977 ApJ 212 743
[7] Luck R E and Bond H E 1980 ApJ 241 218
[8] Luck R E and Bond H E 1989 ApJS 71 559
[9] Smith V V and Lambert D L 1987 MNRAS 227 563
[10] Smith V V and Lambert D L 1986 ApJ 311 843
[11] Cunha K, Sollgren K, Smith V V, Ramirez S V, Blum R D and Terndrup D M 2007 ApJ 669 1011
[12] Larsen S S, Origlia L, Brodie J P and Gallagher III J S 2006 MNRAS 368 L10
[13] Vieira T 1986 Uppsala Astronomical Observatory Report No. 32
[14] Wallace L and Hinkle K 1996 ApJS 107 312
[15] Kurucz R L 1996 ASP Conf Series 108 160
[16] Lundqvist M 2006 PhD Thesis, Lund Observatory
[17] Lundqvist M and Wahlgren G M 2005 Nuclear Physics A 758 304
[18] Kurucz R L 1993 Synthe Spectrum Synthesis Programs and Line Data. Kurucz CD-ROM No. 18
[19] Lambert D L, Brown J A, Hinkle K H and Johnson H R 1984 ApJ 284 223
[20] Wahlgren G M, Robinson R D and Carpenter K G 1992 ASP Conf Series 26 37
[21] Meléndez J and Barbuy B 1999 ApJS 124 527