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## Atomic lines in infrared spectra for ultracool dwarfs<sup>★,★★</sup>

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**Abstract.** We provide a set of atomic lines which are suitable for the description of ultracool dwarf spectra from 10 000 to 25 000 Å. This atomic linelist was made using both synthetic spectra calculations and existing atlases of infrared spectra of Arcturus and Sunspot umbra. We present plots which show the comparison of synthetic spectra and observed Arcturus and Sunspot umbral spectra for all atomic lines likely to be observable in high resolution infrared spectra.

**Key words.** infrared: stars – stars: low mass – brown dwarfs – atomic data

### 1. Introduction

Ultracool dwarfs extend from the cool M dwarfs into the brown dwarf regime and include the spectral types L and T. It is likely that most of the ultracool dwarfs are not massive enough to undergo nuclear fusion in their cores to burn hydrogen and are thus brown dwarfs rather than stars. Here we are concerned in general terms with the spectroscopy of cool objects and use the broad temperature classification “ultracool dwarf” in preference to more specific terms with a physical meaning such as M dwarf and brown dwarf (Jones & Steele 2001).

The astrophysical importance of ultracool dwarf stars derives from the large-scale cosmological significance of their mass density, to their extremely slow chemical evolution and to their formation process and their distinction from planets. Ultracool dwarfs span the mass range from the coolest stars through two orders of magnitude in mass to giant planets. By determining their fundamental parameters, such as effective temperature, metallicity and surface gravity, their position in the Hertzsprung-Russell diagram can be determined. So far these parameters, in particular surface gravity and metallicity,

are poorly determined. Yet to derive a reliable mass function across the brown dwarf regime and to discern the abundance patterns of low-metallicity brown dwarfs, it is essential to design much finer tools of analysis. Changes in effective temperatures, surface gravity and metallicity can lead to similar spectral changes. To disentangle these effects requires observations of several spectral diagnostics that respond differently to changes in these parameters (e.g., Reid & Hawley 2000).

Colour information has proved crucial in the identification of most ultracool dwarfs. However, their complex energy distributions mean that colours do not change monotonically with changing luminosity and temperature. This makes differentiation of second order effects such as metallicity and gravity very difficult to discern. Spectroscopic observations are crucial and low-mass objects have been successfully classified both in the optical (Kirkpatrick et al. 2000; Basri et al. 2000) and infrared (McLean et al. 2001; Geballe et al. 2001; Leggett et al. 2001) regimes across the M and L spectral classes. However by the T spectral class there is insufficient flux at short wavelengths to use optical wavelengths. Furthermore even by the early L spectral class the energy distribution at optical wavelengths is almost completely dominated by broad alkali resonance lines and dust opacities (Pavlenko 1998; Pavlenko et al. 2000; Burrows et al. 2000; Tsuji 2002). The infrared region is also difficult to model with strong molecular opacities of water, iron hydride and at cooler temperatures methane as well. However, there are also a number of atomic lines observable in the infrared spectra of ultracool dwarfs (e.g. McLean et al. 2003). These infrared atomic lines lie across the peak in energy

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\* Figure 1 is only available in electronic form at  
<http://www.edpsciences.org>

\*\* Tables 1 and 2 are only available in electronic form at the CDS  
via anonymous ftp to  
[cdsarc.u-strasbg.fr](http://cdsarc.u-strasbg.fr) (130.79.128.5) or via  
<http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/416/655>

distribution for these stars and are thus comparatively easier to observe than lines of the same atoms in the visible.

In recent years there has been a focus on improvements to the atomic data in the optical region, e.g., NIST (Kelleher et al. 1999), Opacity Project (Seaton et al. 1992). However, currently the accuracy and completeness of the atomic data, in particular oscillator strengths, in the IR region are far poorer. In many cases either the oscillator strengths are highly inaccurate or there are simply no measurements available. This becomes evident when synthetic spectra are generated to match infrared spectra, e.g., Jones et al. (1996), Jones & Viti (2000). Here we identify suitable sensitive infrared atomic lines that may one day be used for reliable temperature, gravity and abundance analyses for a wide range of ultracool dwarfs, from M dwarf stars through brown dwarfs as well as extra-solar giant planets. Our paper is the first step in the development of a database of infrared atomic lines with reliable oscillator strengths suitable for the study of low temperature astrophysical objects. Our specific focus is the interpretation of ultracool dwarfs covering the temperature space from the M dwarfs through the brown dwarfs to extra-solar giant planets.

Our focus is the prioritisation of atomic lines whose oscillator strengths we are either already measuring or planning to measure. Section 2 describes the observational material, atomic line lists and theoretical spectra necessary for this study. Our procedures for identifying important infrared atomic transitions are discussed in Sect. 3. In Sect. 4 we discuss our results and conclusions. In Sect. 5 we outline our plans for experimental measurements of the atomic data.

## 2. Input datasets

### 2.1. Observed spectra of Arcturus and Sunspot umbra

For comparisons and the robust identification of atomic lines we used both electronic and hard copies of the “Infrared Atlas of the Arcturus spectrum, 0.9–5.3  $\mu\text{m}$ ” (hereafter “Arcturus atlas”) (Hinkle et al. 1995) and “An Atlas of a Dark Sunspot Umbral spectrum from 1970 to 8640  $\text{cm}^{-1}$  (1.16 to 5.1  $\mu\text{m}$ )” (hereafter “Sunspot umbra atlas”) (Wallace & Livingston 1992). We used the electronic versions of both atlases (<ftp://ftp.noao.edu/catalogs/arcturusatlas/ir/> and <ftp://ftp.noao.edu/fts/spot1at1/>) to compare with our synthetic spectra.

Arcturus ( $\alpha$  Boo) is a K1 III star of effective temperature  $T_{\text{eff}} = 4300 \pm 30$  K and  $\log g = 1.5 \pm 0.15$  (Peterson et al. 1993). These parameters are far from adequate to describe ultracool dwarf atmospheres ( $T_{\text{eff}} \leq 2600$  K,  $\log g \sim 4.5$ – $5.0$ ) though the Arcturus atlas provides careful identification of atomic lines and gives an opportunity to assess the behaviour of atomic lines when decreasing effective temperature from 4000 K to 2000 K. The atlas contains winter and summer observations. Since only the telluric spectrum is affected by seasons, in this paper we only use the telluric free summer data. The resolution of this atlas is of the order of  $R \sim 100\,000$ . The presence of a magnetic field in Arcturus is indirectly confirmed by strong emission lines in the ultraviolet spectral region formed in chromosphere of Arcturus (Ayres et al. 1986). However the average

value of the magnetic field is, probably, similar to the solar one, since atomic line splitting is not seen in the observed spectrum.

The Sunspot umbra atlas has a spectral type of M2–M5 V, which corresponds to an effective temperature range of around  $T_{\text{eff}} = 3170$ – $3520$  K (Wallace & Livingston 1992; Viti et al. 1998). The magnetic field strength is estimated as  $\approx 3360$  Gauss. Due to the position of the umbra near the centre of the solar disk we see only  $\sigma$ -components of Zeeman split lines of large Lande factor  $g$  in the Sunspot umbra atlas. Due to the strong magnetic field in the spot most of the atomic lines in the Sunspot umbral spectrum have doublet-like profiles. Molecular lines, with few exceptions, are magnetically insensitive and show single profiles. The Sunspot umbra atlas provides a spectrum corrected for atmospheric absorption. Its resolution is  $R \sim 200\,000$  between 10 000 and 25 000  $\text{\AA}$ .

### 2.2. Synthetic spectra

Computations of synthetic spectra were carried out using the WITA6 program (Pavlenko 2000) assuming Local Thermodynamic Equilibrium.

For the computation of synthetic spectra we used the NextGen model atmospheres structures (Hauschildt, private communication; Hauschildt et al. 1999) for cool spectra, and model atmosphere structures of Kurucz (1994) for the higher temperature synthetic spectra of Arcturus.

The atomic linelist used for our spectral modeling and line identification was taken from the VALD database (Kupka et al. 1999). VALD is a compilation of several different lists of atomic line data which were obtained from experimental measurements and theoretical calculations by various authors.

Chemical equilibria were computed for the mix of around 100 molecular species. Input molecular data and continuum opacity sources are described elsewhere (Pavlenko et al. 1995; Pavlenko 1997, 2000). The profiles of absorption lines are described by the Voigt function  $H(a, \nu)$ . The formulae of Unsold (1955) were used for calculation of damping constants. For these model atmospheres we adopt the conventional value of microturbulent velocity  $v_t = 2$   $\text{km s}^{-1}$ . Theoretical spectra were computed with a wavelength step of 0.05  $\text{\AA}$  and then convolved with Gaussians to match the instrumental broadening.

We should note, that we didn’t consider dusty effects in our synthetic spectra calculations, since the main purpose of the present work was not to model the real spectra of ultracool objects, but to reveal the prominent atomic features to be observed in such objects. The effects of dust will modify atomic line strengths in ultracool dwarf spectra. But dust will not affect the quantum-mechanical parameters which we intend to measure at the present time.

## 3. Procedure

Our procedure of line identification and selection is based on the comparison of synthetic spectra with the observed spectra of Arcturus and Sunspot umbra from 10 000 to 25 000  $\text{\AA}$ .

For ultracool dwarfs we used only synthetic spectra. The choice of model atmosphere parameters was aimed at obtaining

a reliable atomic line list for ultracool dwarfs in the IR region. A model atmosphere of  $T_{\text{eff}}/\log g/[M/H] = 2000/5.0/0.0$  was selected (hereafter “ultracool dwarf model”). This corresponds to an ultracool dwarf spectral class of around L0 (Kirkpatrick et al. 1999; Martin et al. 1999). The half width of the Gaussian we used to account for instrumental broadening in the “ultracool dwarf” synthetic spectrum is  $0.4 \text{ \AA}$  which corresponds to resolution  $R \sim 20\,000\text{--}40\,000$ , approximately the resolution available to modern infrared echelle spectrometers operating between  $10\,000\text{--}25\,000 \text{ \AA}$ . Another model atmosphere  $4000/4.5/0.0$  (hereafter “Arcturus-like model”) was chosen to select some observable spectral atomic features formed in hotter atmospheres. The half width of the Gaussian for this synthetic spectrum is  $0.13 \text{ \AA}$  to match the line broadening by macroturbulent velocity  $v_{\text{macro}} = 3.5 \text{ km s}^{-1}$  in the Arcturus spectrum (Peterson et al. 1993). The  $T_{\text{eff}} = 4000 \text{ K}$  is slightly lower than Arcturus  $T_{\text{eff}} = 4300 \text{ K}$  (Peterson et al. 1993), and higher than the temperature of the Sunspot umbra  $T_{\text{eff}} \sim 3170\text{--}3520 \text{ K}$  (Wallace & Livingston 1992).

In the electronic versions of the Arcturus and Sunspot umbra atlases the data are given on a wavenumber scale. We transform the wavenumbers to wavelengths in air using the formula from Allen’s *Astrophysical Quantities* (2000).

It is well known that the difficulties of line identification in IR spectra of ultracool dwarfs have a number of causes. There are many strong molecular lines of  $\text{H}_2\text{O}$  (Jones et al. 2002),  $\text{FeH}$  (Cushing et al. 2003),  $\text{CO}$  (Pavlenko & Jones 2003),  $\text{CH}_4$  (Noll et al. 2000) native to ultracool dwarfs as well as telluric molecular lines, particularly strong between the *J*, *H* and *K* bands. Nevertheless, we were able to identify many absorption features in the atmospheres of Arcturus and Sunspot umbra spectra likely to be present in ultracool dwarfs. To do this, we developed a procedure based on the inter-comparison of computed and observed spectra designed to minimise possible errors in line identification. The line identification files were made using:

- a) “ultracool dwarf” synthetic spectrum (2000/5.0/0.0);
- b) “Arcturus-like” synthetic spectrum (4000/4.5/0.0).

In addition we used line identification files from hard copy Arcturus and Sunspot umbra atlases.

In our identification procedure we assume that lines absorb only at a given wavelength. This assumption provides an upper limit of absorption. In the real spectra the residual intensity may be lower due to contribution of other lines. For every line from the VALD linelist in the range of  $10\,000\text{--}25\,000 \text{ \AA}$  the residual flux  $r_{\nu} = \frac{(\text{Flux in line})_{\nu}}{(\text{Flux in continuum})_{\nu}}$  was computed. Atomic lines from VALD with central intensities deeper than 0.8 of the residual flux in the spectrum of 2000/5.0/0.0 atmosphere were selected to restrict the number of lines to those likely to be observable in cool spectra. These lines are given in the Table 1. The set of the selected lines is rather large and thus we assign different levels of priority to the lines. The main criteria for selecting lines of the highest priority is that the central intensity of the identified line ought to be greater than 0.6 of the residual flux (Col. 4 in the Table 1) in the “ultracool dwarf” synthetic spectrum.

Plots for all spectral regions containing atomic lines of interest are shown in Fig. 1 (they are also

available at <http://www.astro.livjm.ac.uk/~hraj/spectralatlas/index.html>). The identifications of atomic features are labelled in the spectra. Arrows and labels at the top of the plots show identification in the “ultracool dwarf” synthetic spectrum, the same labels in the bottom of the plots are for the “Arcturus-like” spectrum. The Sunspot umbra spectrum is shown by bold line, the Arcturus spectrum by a dotted line, the “ultracool dwarf” synthetic spectrum as a solid line and “Arcturus-like” synthetic spectrum as a dashed line. In order to simplify our plots molecular line identifications are not included. Usually molecular lines have narrow deep profiles allowing them to be distinguished from atomic lines. Their identification in the Sunspot umbra and Arcturus can be found in the hard copy atlases.

## 4. Results

Our results are shown in two tables. Table 1 contains all identified lines with central intensities deeper than 0.8 of residual flux using “ultracool dwarf model” identifications. Table 2 investigates the sensitivity of priority 1 lines identified in Table 1 to temperature, gravity and metallicity.

In the first column of Table 1 we estimate the priority of lines for measurement of atomic data.

- a) Priority 1 indicates that the atomic line is deeper than 0.6 in the 2000/5.0/0.0 synthetic spectrum. Also we include as first priority three lines of Ti (22211.229, 22232.838, 22274.012  $\text{ \AA}$ ) which are shallower than 0.6. They are located far from strong atomic and molecular lines and thus are good for identification purposes in the spectra of ultracool dwarfs.
- b) Priority 2 indicates that the residual flux of an atomic line is between 0.8–0.6.
- c) Priority 3 indicates that the atomic line is located in the wing of a nearby stronger line or in a wavelength region with strong telluric absorption.

Atomic lines without an assigned priority might be relevant in the analysis of ultracool dwarf spectra, but they are predicted to be weak in the synthetic spectrum.

The second column shows the wavelength of the line in  $\text{ \AA}$  in air. These values were taken from VALD. We check that wavelengths from Arcturus and Sunspot umbra atlases identification files are in a good agreement with VALD. The wavelengths of a few lines differ from VALD values by less than  $0.1 \text{ \AA}$  in the region  $10\,000\text{--}20\,000 \text{ \AA}$  and by less than  $0.3 \text{ \AA}$  beyond  $20\,000 \text{ \AA}$ .

The third column shows the atomic identifications of the line.

Columns 4–7 show the linedepths of identified lines. Column 4 – the residual flux in the line obtained from the “ultracool dwarf” synthetic spectrum; Col. 5 – from the “Arcturus-like” synthetic spectrum; Col. 6 – measured from the hard copy of Arcturus atlas depth of identified atomic lines; Col. 7 – the same as Col. 6 for the hard copy of the Sunspot umbra atlas. As was mentioned above we used the hard copy versions of the Arcturus and Sunspot umbra atlases to measure linedepths.

The accuracy of our line depth measurements from the hard-copy atlases is  $\sim 0.01$ – $0.02$  for the Arcturus atlas (Col. 6) and  $\sim 0.02$ – $0.03$  for the Sunspot umbra atlas (Col. 7). We note that linedepth information given in Cols. 6 and 7 is only used to check the presence of a line in the observed spectra. Thus we do not need high accuracy linedepth measurements for the observable spectra of the Sunspot umbra and Arcturus.

We note that the data in the Sunspot umbra atlas provide a spectrum from  $11\,600\text{ \AA}$ , rather than  $10\,000\text{ \AA}$  where our figures and tables start from. Some lines are labelled (see Col. 7) by the symbol “~” which means that part of the line in the hard copy of the atlas is obscured by a gap in the data and the value given in the table is for the visible part of the line. In Cols. 6 and 7 there are also some lines with “bl” suffices. This means that these lines are blended with stronger nearby lines.

There are two regions with strong telluric absorption (marked in Cols. 6 and 7 by  $\oplus$ ):  $13\,600$ – $14\,770\text{ \AA}$  and  $18\,260$ – $19\,450\text{ \AA}$ , regions between the *J* and *H*, and *H* and *K* photometric bands. Lines identified from VALD in these regions are difficult to observe in ground based observations but can be used in probable future space observations of ultracool dwarfs.

Finally we note, that in Table 1 we italicise atomic lines of Rb, Y, Ba and Lu, identified only using theoretical computations. Although these lines are not seen in the observations of Arcturus and Sunspot umbra, they are strong in the synthetic spectrum computed for the 2000/5.0/0.0 model atmosphere, and therefore also likely to be strong below 2000 K.

In Table 2 we show only lines which were marked in Table 1 as first priority lines. The first column are wavelengths in  $\text{\AA}$ ; the second column are names of elements. In the third column we give the central line intensity for the “ultracool dwarf” (2000/5.0/0.0) spectrum. We compute some synthetic spectra for ultracool objects varying parameters of  $T_{\text{eff}}$ ,  $\log g$  and metallicity to show the sensitivity of the central intensities of identified lines to these parameters. For our computations we chose the minimal step in model atmospheres grid:  $\Delta T_{\text{eff}} = 100\text{ K}$ ,  $\Delta \log g = 0.5$ ,  $\Delta [M/H] = -0.5$ . In Cols. 4–6 we show the difference of central intensity (in %) computations with “new” models from central intensity computations for our “ultracool dwarf model”. Negative values in Cols. 4–6 indicate that a line is stronger in the new model relative to the reference model 2000/5.0/0.0.

Column 4 shows the dependence of residual fluxes on effective temperature. For comparison a 2100/5.0/0.0 synthetic spectrum was used. One can see that only a few lines show strong temperature dependence for  $\Delta T_{\text{eff}} = 100\text{ K}$ . The NextGen 2000/4.5/0.0 model was used with 2000/5.0/0.0 to test gravity sensitivity. The dependence for  $\Delta(\log g) = 0.5$  is also relatively weak for most lines and is shown in Col. 5.  $\Delta [M/H] = 0.5$  from computations using NextGen model atmospheres 2000/5.0/-0.5 and 2000/5.0/0.0 is shown in Col. 6. The metallicity dependence is relatively high for all lines. Thus Table 2 indicates that relatively small variations of model atmosphere parameters will not seriously affect our line selection and prioritisation.

## 5. Experimental work

The identification and prioritisation of atomic lines presented in this paper is only the first step in our project and is primarily based on a theoretical treatment. Our program of measurements of atomic data for the priority lines given in this paper is underway. We are currently measuring oscillator strengths by measurements of sets of relative line intensities using the high resolution Fourier transform spectrometers at Imperial College (Pickering 2002) and NIST (National Institute of Standards and Technology, US). We have already recorded spectra of Ti, Mn and Na, and measurements of Mg, K, Ca and Fe are in progress. Measurements of other species listed in Table 1 are underway in the near future. These line intensities will be used to obtain branching ratios which are then combined with level lifetimes to obtain *f*-values. We expect to achieve uncertainties in *f*-values of around 10–15%.

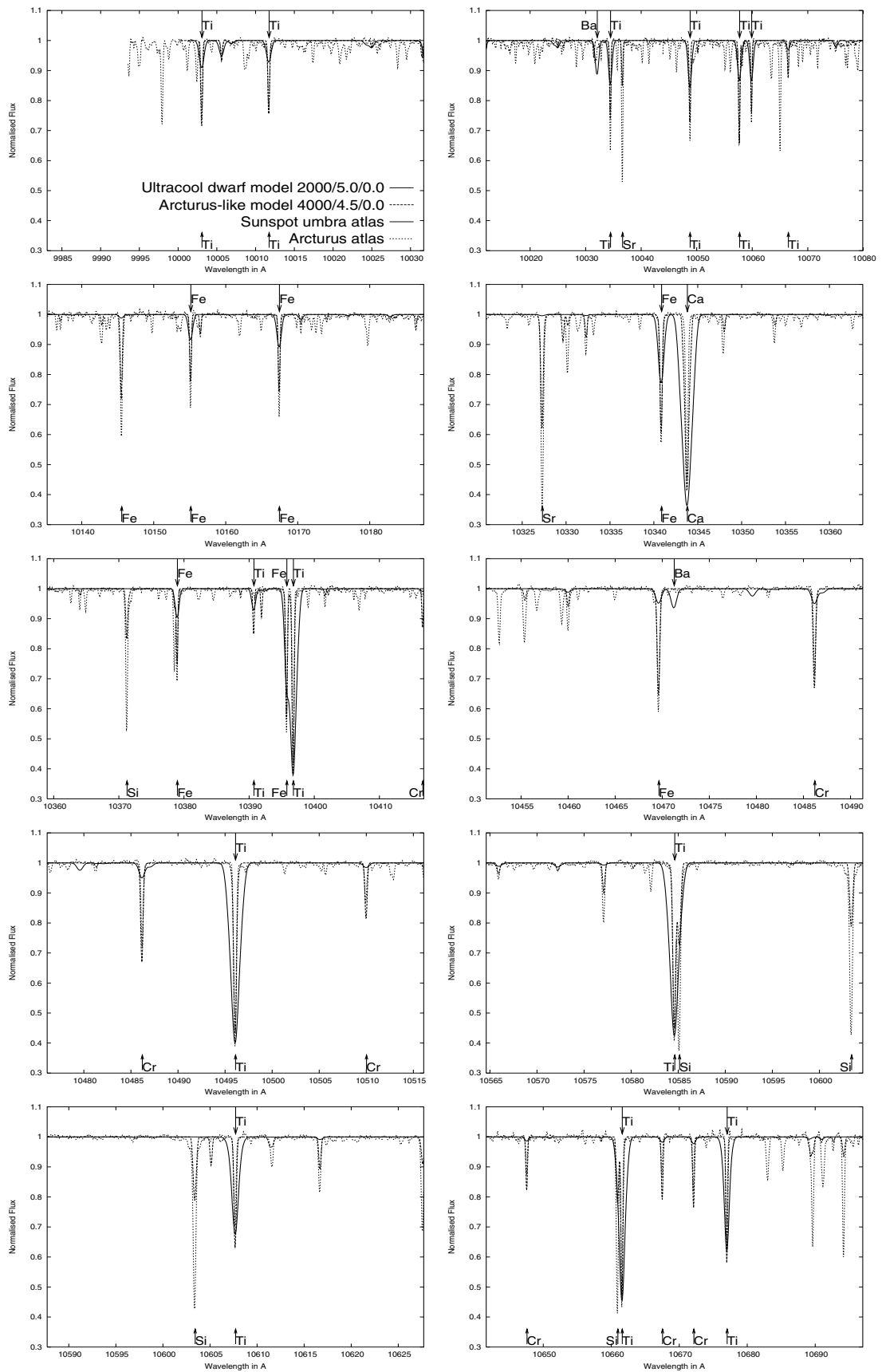
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**Fig. 1.** Plots for all spectral regions containing atomic lines of interest in the 10 000–25 000 Å region. The identifications of atomic features are made by atomic name and arrows by the line of interest. Identification at the top of the plots is for the “ultracool dwarf” spectrum; identification at the bottom of the plots is for the “Arcturus-like” spectrum.

