*Article*

# Application of Laboratory Atomic Physics to Some Significant Stellar Chemical Composition Questions

**Christopher Sneden**[1] 0000-0002-3456-5929, **James E. Lawler** [2] **and Michael P. Wood** [3]*

1   Department of Astronomy and McDonald Observatory, The University of Texas, Austin, TX 78712;
    chris@verdi.as.utexas.edu
2   Department of Physics, University of Wisconsin-Madison, 1150 University Ave, Madison, WI 53706, USA;
    jelawler@wisc.edu
3   Department of Physics, University of St. Thomas, 2115 Summit Ave, St. Paul, MN 55105, USA;
    mpwood@stthomas.edu
*   Correspondence: chris@verdi.as.utexas.edu; Tel.: +1-512-471-1349

1   **Abstract:** This brief review highlights some current issues in Galactic stellar nucleosynthesis, and
2   some recent laboratory studies by the Wisconsin atomic physics group that have direct application
3   to stellar spectroscopy, in order to advance our understanding of the chemical evolution of our
4   Galaxy. The relevant publication history of the lab studies are summarized, and investigations into
5   the abundances of neutron-capture and iron-peak elements in low metallicity stars are described.
6   Finally, new initatives in near-infrared spectroscopy are briefly explored.

7   **Keywords:** atomic physics, transition probabilities, hyperfine and isotopic substructure, stellar
8   spectroscopy, chemical compositions

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9   **1. Introduction**

10      15 years ago the United States National Academy of Sciences suggested a set of "Eleven Science
11  Questions for the New Century" [1]. One consideration deemed worthy of inclusion in that list
12  was, "How Were the Elements from Iron to Uranium Made?" This question sums up the overall
13  goals of many efforts in fields labeled variously as Galactic chemical evolution, stellar nucleosyntheis,
14  and cosmochronology. Most information for these fields must come from stellar surface chemical
15  compositions, with additional contributions from solar system meteoritics, planetary nebulae, $H_2$
16  regions, and supernova remnants.

17      The basic tool for stellar elemental abundance studies is spectroscopy, generally obtained with
18  wavelength resolving power comparable to the widths of stellar absorption lines. Most of the stars
19  investigated for clues to nucleosynthesis are relatively cool, with effective temperatures $T_{eff} < 10,000$ K.
20  Their spectra are comprised almost entirely of neutral and singly-ionized species of elements with
21  atomic numbers $Z \geq 6$ and diatomic molecules mostly involving the HCNO elements. Their surface
22  chemical compositions reflect the combination of elements synthesized and ejected into the interstellar
23  medium by past stellar generations, and elements produced in the interiors of the stars themselves.

24      Determination of accurate elemental abundances from atomic lines in stellar atmospheres involves
25  many areas of physics and astronomy, including laboratory and theoretical atomic physics, statistical
26  and thermal physics, construction of realistic model stellar photospheres, solutions to the radiation
27  transport problem due to a variety of absorption and scattering processes, details of stellar line
28  formation, etc. Limits on the abundance accuracies can arise from multiple sources, and any weak link
29  in the analysis chain can potentially destroy the usefulness of an element in helping to understand

30  nucleosynthesis. The quest for more accurate stellar abundances must start with the parameters of
31  individual atomic transitions. One must know their quantum properties very well, including their
32  transition probabilities and isotopic and hyperfine substructures, to have any hope of deriving robust
33  abundances from them. Our collaboration from The University of Wisconsin at Madison and The
34  University of Texas at Austin has concentrated on improving these basic line parameters through
35  laboratory experiments, and applying these lab data to classes of stars most relevant to Galactic
36  chemical evolution descriptions.
37      Several atomic physics groups are making major contributions to improving transition data
38  through many theoretical and laboratory approaches. These groups and some representative
39  publications include, but are not limited to, those at: The University of Mons [2,3]; Imperial College
40  London [4,5]; Lund University [6,7], and Uppsala University [8,9]. This paper aims to highlight the
41  University of Wisconsin laboratory studies of atomic species most relevant to cool-star spectroscopy.

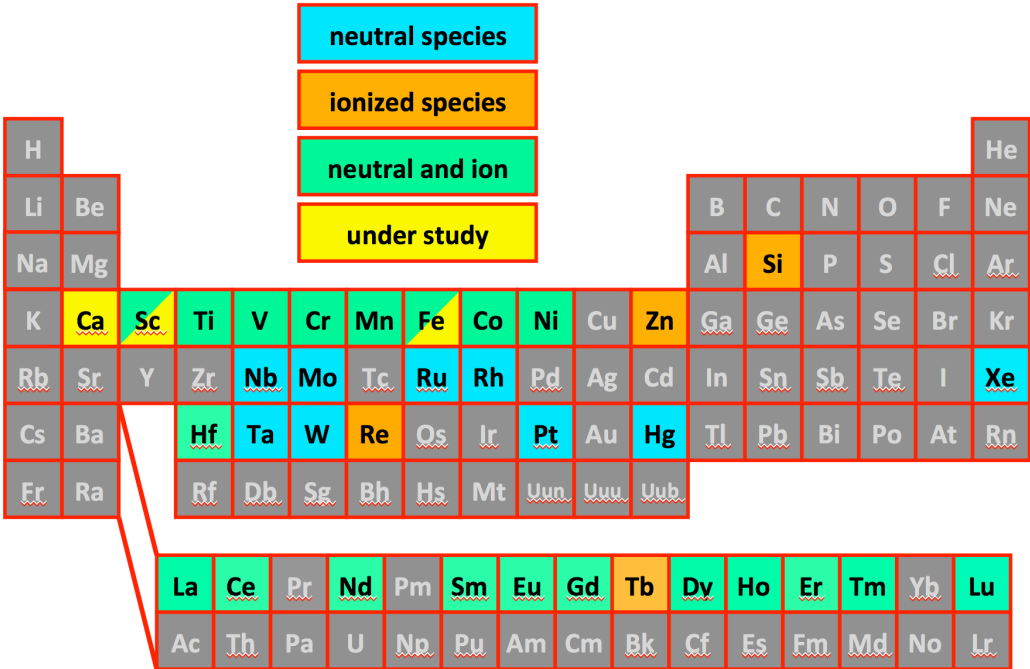42  **2. Laboratory Transition Data**



**Figure 1.** A periodic table color-coded by published neutral and ionized species laboratory transition probabilities from the Wisconsin group. The elements shown in gray boxes have not been studied; the blue, orange, green and yellow colors are defined in the figure.

43  Two important astrophysical element groups have been featured: the Fe-peak elements
44  ($21 \leq Z \leq 30$), and the neutron-capture (*n*-capture) elements ($Z > 30$). In Figure 1 we show in
45  periodic table format the elements with published Wisconsin lab $gf$ values, color-coded by the species
46  that have been studied. Except for Xe I [10] and Ni II [11], all of the results include transitions that are
47  readily accessible in the optical ($3000-9500$ Å) and ultraviolet ($UV$: $2200-3000$ Å) spectral domains of
48  cool stars.[1] There are many individual studies, and here we comment on a few aspects of these lab
49  investigations.

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1    Only the Xe I 1470 Å resonance line was investigated by [10]; seven Ni II lines in the $1450-1750$ Å were included by [11].

Of primary importance is the ability of stellar spectroscopists to have access to single-source internally consistent transition data for as many lines as possible for a given species. A few decades ago stellar abundance studies had to rely on a patchwork set of relatively inaccurate lab and theoretical line parameters, or to resort to differential analyses of stellar and solar spectra. Neither of these approaches could produce abundances that are accurate enough to meaningfully compare to stellar nucleosynthesis predictions. Happily, the huge increase in quality and quantity of transition data means that for most spectroscopically-accessible species the basic line data are now very small factors in abundance error budgets.

Among the Fe-group elements, accurate transition probabilities have been published recently for Fe I [4,12,13] through the combined efforts of the groups at Imperial College London, Uppsala, and Wisconsin. Almost all of the transitions reported in these papers arise from states with lower excitation energies $\chi > 2.2$ eV. For Fe I lines with smaller excitation energies, the older lab study of [14] still provides trustworthy transition probabilities. Combining lab data from these studies and applying them to the solar photosphere and metal-poor stars appears to yield reliable Fe abundances with relatively small line-to-line scatter [15]. Unfortunately, no single comprehensive lab study of Fe II has been published recently; see the summary of sources up to 2016 in [15].

The neutral species for Ti through Ni have been extensively studied [16–21], and the ionized species for these elements except Ni (see above footnote) [19,22–25]. Application to the solar photospheric spectrum and to the spectrum of the well-studied metal-poor field star HD 84937 results in accurate, internally consistent abundances for each species. More importantly, the abundances for both species (when available) are in agreement (see Figure 7 of [15]), strongly suggesting that the derived Fe-group abundances are true chemical composition markers, relatively unaffected by line formation and stellar atmospheric modeling uncertainties.

An earlier series of lab studies concentrated on near-complete coverage of the ionized species of "rare earth" lanthanides. Only the ionized species of lanthanides are usually detectable is stellar spectra. In spite of their relatively small abundances in most stars in comparison to the Fe-peak group, there are many ionized-species lanthanide lines detectable in the blue and near-*UV* spectrum of cool stars. In Figure 1 it is clear that most Wisconsin lab studies of *n*-capture elements outside the lanthanide domain have been on neutral-species transitions. In many cases this mirrors their stellar spectroscopic accessibility. Neutral species lines of these elements mostly are few and far between, and rarely do ionized species lines become detectable.

### 3. Some Applications of Laboratory Data to Low Metallicity Stars.

The onset of Galactic nucleosynthesis produced stars of very low overall metallicity[2] and many of these objects exhibit large departures from the solar-system abundance distribution. Among the *n*-capture elements there are outstanding examples of stars that have been born with or acquired from a companion extreme enhancements of elements (isotopes) that were generated in fusion environments that were conducive to slow neutron captures (the *s*-process) or rapid-blast ones (the *r*-process).

There has been renewed interest in the *r*-process production site following the recent discovery of gravitational wave event GW170817, so far unique in providing electromagnetic signals as well in multiple wavelength domains. The totality of "multi-messenger" information from GW170817 strongly suggests that this event arose from the merger of two neutron stars [27]. Additionally, photometric and spectroscopic observations [28,29] suggest the presence of *r*-process-rich ejecta from this event, in particular of unstable lanthanide isotopes. It is important to determine accurate abundances for as many *n*-capture elements in *r*-process-rich stars as possible to quantitatively constrain what the output of a binary neutron star merger must match.

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[2]  We adopt the standard spectroscopic notation [26] that for elements A and B, $[A/B] \equiv \log_{10}(N_A/N_B)_\star - \log_{10}(N_A/N_B)_\odot$. We use the definition $\log \epsilon(A) \equiv \log_{10}(N_A/N_H) + 12.0$, and equate metallicity with the stellar [Fe/H] value.

The first extremely *r*-process-rich star, CS 22892-052, was recognized on a noisy high-resolution spectrum and analyzed with weak laboratory data [30]. A total of 54 lines contributed to abundances of 12 *n*-capture species. Contrast that with the study of the recently-discovered *r*-process-rich star J09544277+5246414 [31], which reported abundances based on 134 lines of 28 species. In Figure 2 we reproduce their comparison of abundances of that star and scaled solar-system *r*-process-only abundances. The match is near-perfect in the lanthanide domain, and it is in many other *r*-process-rich stars, e.g., [32,33]. Spectroscopically this means that atomic data parameters for a large number of detectable *n*-capture elements are now good enough that they play only a very small part of the overall elemental abundance uncertainties. Astrophysically this means that the creation of *r*-process elements has been essentially the same over Galactic history, and possibly limited to one type of production site.
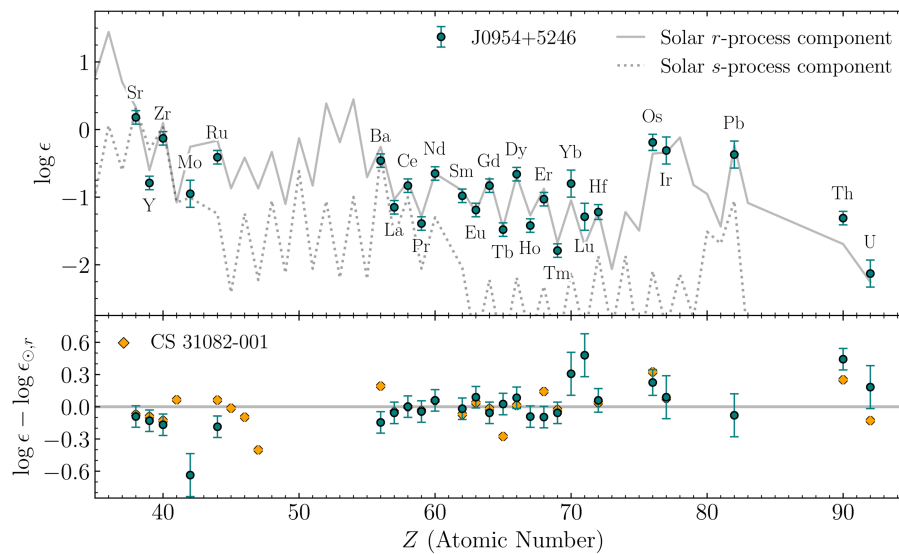


**Figure 2.** Abundances of *n*-capture elements in the very metal-poor *r*-process-rich star J0954+5246 and those of *r*-process and *s*-process material in the solar system [31]. In the top panel the abundances are presented, and in the bottom panel the differences between the star and solar *r*-process-only abundances are shown.

For low metallicity stars the Fe-group element abundances have not had the same level of atomic physics attention as the *n*-capture elements. It has been known for decades that relative abundances among this element group do not conform exactly to the solar-system distribution [34–36]; [Mn/Fe] < 0 and [Cu/Fe] < 0. Additionally, [37,38] suggested that below metallicity levels of [Fe/H] $\sim -2.5$ there are decreases in [Cr/Fe] and increases in [Co/Fe], yielding [Co/Cr] $\sim +1$. However, these results have generally depended on very few transitions of the neutral (minority) species of Mn, Cr, Co, and Cu. Recently, with the new Wisconsin lab transition data discussed in §2, a large study of a warm metal-poor ([Fe/H] $\sim -2.3$) unevolved "main sequence" turnoff star [15] included these features:

- continuous spectral coverage from the *UV* through the optical, 2300−8000 Å;
- ∼550 Fe I and Fe II lines, ∼600 lines of other Fe-group neutral and ionized species ([15] Figure 1);
- precise abundances from 17 Fe-peak species, with good agreement between neutrals and ions of seven elements ([15] Figure 7);
- little sign of over-ionization of neutral species, which would be a signature of departures from local thermodynamic equilibrium (LTE) in the Fe-group neutral species;
- no evidence for depletion of Cr and enhancement of Co at this metallicity;
- a curious overabundance of the three lightest Fe-peak elements Sc, Ti, and V.

This work is being extended to lower metallicities [39,40] to investigate Fe-peak abundance ratios for any solid evidence of other departures from the solar-system distribution.
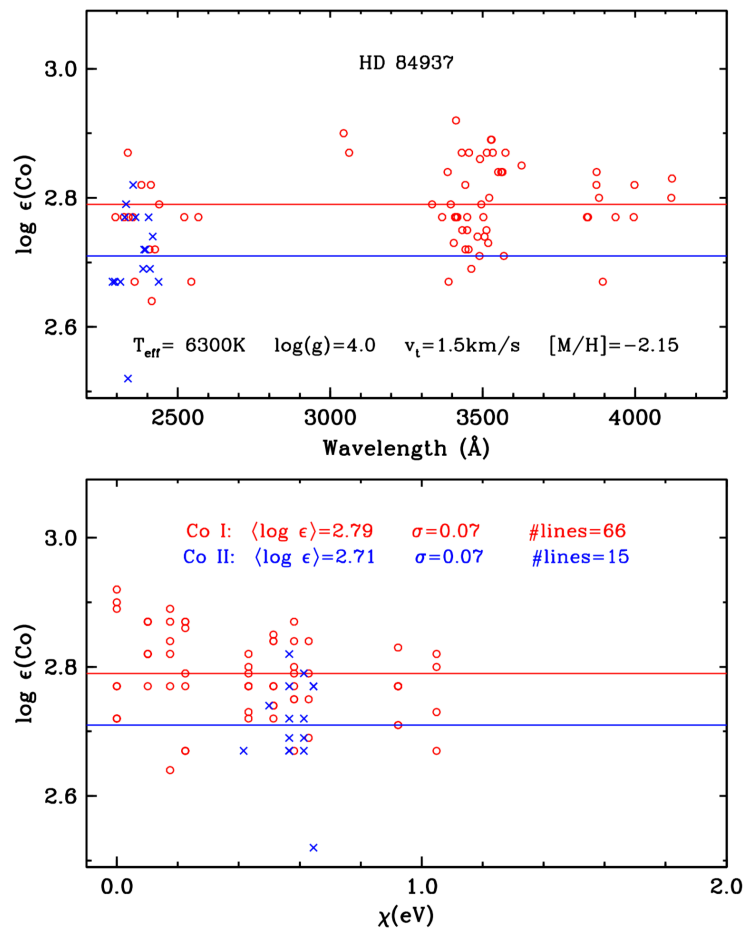
**Figure 3.** Abundances of Co I (red circles) and Co II (blue x's) lines in HD 84937 as functions of wavelength (top panel) and excitation energy (bottom panel), taken from [24].

123      Lab studies of Fe-peak elements are continuing. The HD 84937 study detailed above did not
124 include recent transition studies of Sc II, Cr II, Co II, Cu I or Zn I. New data for Cr II [23] yields
125 consistent abundances from neutral and ionized species in the solar photosphere. The same agreement
126 is seen HD 84937 as long as the anomalously small abundances (0.2-0.3 dex lower than the rest of the
127 Cr transitions) from the Cr I resonance lines at 4254, 4274, and 4289 Å are ignored. This appears to be a
128 clear signal of departures from LTE in the neutral species. We suspect that this may explain the earlier
129 reports of Cr deficiencies in very metal-poor stars, since the Cr I resonance lines have played a major
130 role in most Fe-peak abundance surveys.
131      Recently [24] have reported new lab data for Co II transitions, almost all of which arise in the $UV$
132 spectral region. In Figure 3 we summarize the HD 84937 abundances from that study. Translating these
133 $\log \epsilon$ values into relative abundances with respect to the Sun yields [Co/H] = $-2.24$ or [Co/Fe] =$+0.08$,
134 essentially the solar ratio within the observational uncertainties. There is no obvious enhancement in
135 the relative Co abundance at this metallicity. Interestingly, the abundance from Co I lines is 0.08 larger;
136 one looks for over-ionization of an element as evidence for non-LTE effects, but in HD 84937 we derive
137 an *under*-ionization. This anomaly is being further tested with our more metal-poor stellar sample
138 [39,40]; preliminary evidence supports the notion that Co is not overabundant in very metal-poor stars,
139 i.e., [Co/Fe] $\sim 0$ for stars with [Fe/H] $\leq -3$.
140      The vacuum-$UV$ spectral region, $\lambda < 3000$ Å, presents the ideal stellar laboratory to make progress
141 in understanding Fe-peak abundances in low metallicity stars. Hundreds of potentially useful neutral
142 and ionized species transitions can be easily identified in the vacuum $UV$. Unfortunately the required
143 high-resolution spectra may only be acquired with the Hubble Space Telescope *STIS* instrument.

144 At present there are less than about 20 metal-poor ([Fe/H] $< -2$) stars with good $HST/STIS\ UV$
145 spectra. Given the ongoing demand for $HST$ time, one cannot reasonably expect a large expansion
146 of this meager data base. A more feasible goal will be to use ground-based large telescopes with
147 good near-$UV$ high resolution spectrographs (e.g., $VLT/UVES$, $Keck/HIRES$) to access more Fe-peak
148 transitions in the 3000-4000 Å spectral range.

## 4. Extending the Wavelength Domain to the Near-Infrared

150 The near-infrared spectral domain, $1.0-2.4\ \mu$m, is enjoying new high-resolution spectroscopic
151 access, with such telescope/instrument combinations as $VLT/CRIRES$, $SDSS/APOGEE$, and
152 $McDonald - DCT - Gemini/IGRINS$ now able to provide quality spectra of many faint ($K \leq 14$)
153 targets in star clusters, the general Milky Way field and the Galactic bulge. Laboratory atomic
154 physics so far has not been able to keep pace in the near-$IR$, mostly due to intrinsic difficulties in
155 deriving accurate atomic transition probabilities. Upper levels that only radiate in the infrared ($IR$)
156 are not currently accessible to TRLIF (Time-Resolved Laser-Induced Fluorescence) radiative lifetime
157 measurements. The lack of an IR equivalent to an optical-UV photomultiplier ($PMT$) is a problem.
158 The combination of $PMT$ gain, electronic bandwidth, and detector area is not yet available in the $IR$.
159 Progress is needed, and here we describe some aspects of the efforts of the Wisconsin group in this
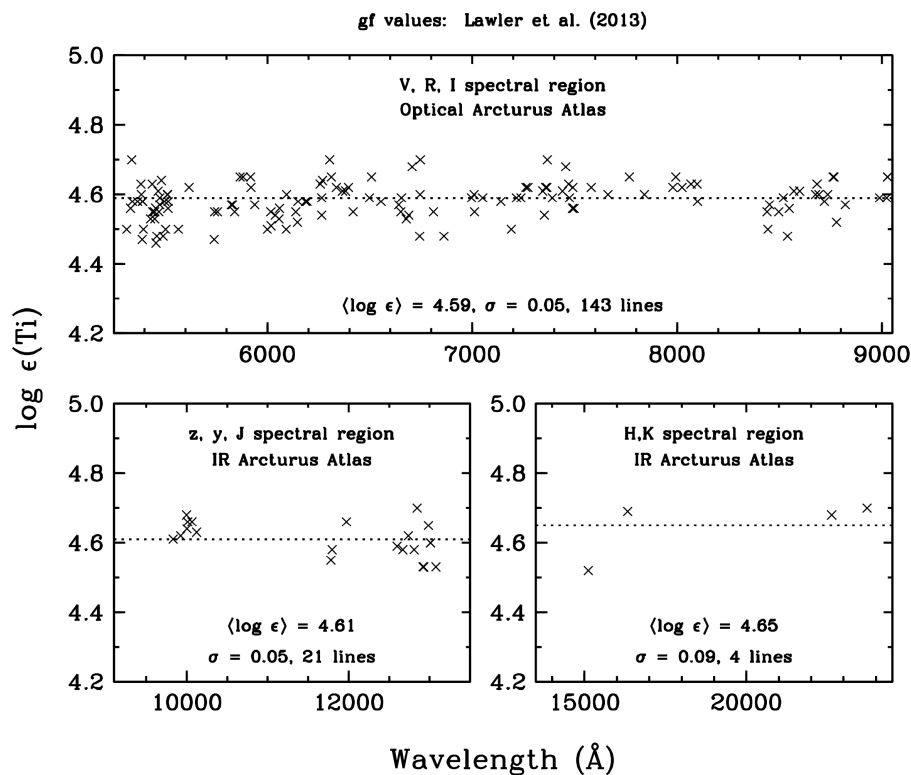160 spectral domain.



**Figure 4.** Abundances of Ti in the well-studied red giant Arcturus from Ti I lines in the optical and near-$IR$ spectral domains. The top panel shows results from the optical region defined by astronomical photometric bands $V$, $R$, and $I$, while the two bottom panels show near-$IR$ spectral regions $z$, $y$, and $J$ (left), $H$ and $K$ (right). Obvious wavelength gaps with no Ti I line abundances are mostly due to telluric molecular absorption blocking starlight from reaching the ground.

161 [16] reported accurate transition probabilities for nearly 950 Ti I lines, and derived new Ti
162 abundances for the solar photosphere and very metal-poor star HD 84937. However, the absorption
163 strengths of Ti I lines, like those of most species, decrease substantially with increasing wavelength,

164  and there are relatively few measurable ones in warm stars like the Sun and especially in metal-poor
165  stars. Such stars cannot be used to test the parameters of many atomic lines redward of ∼8000 Å.
166  For this task we have recently turned to the bright, mildly metal-poor ([Fe/H] ≃ −0.5) red giant
167  star Arcturus. This star has both excellent high-resolution spectroscopic atlases and careful model
168  atmosphere studies. The reader is referred to [41] for citations to these studies and a discussion of V I
169  transitions in the red spectral region of Arcturus.

170      In Figure 4 we present abundances for 168 Ti I lines in Arcturus from 5200 Å to 2.4 $\mu$m. The mean
171  abundance, log $\epsilon$(Ti) ≃ 4.6, suggests that [Ti/H] ≃ −0.4 or [Ti/Fe] ≃ +0.1. The transition probabilities
172  for these analyses all come from [16], and in general they yield a consistent Ti abundance. There is
173  a very small upward drift in derived abundances with increasing wavelength, but it may arise from
174  a variety of possible causes. The important conclusion is that for Ti I the optical and near-*IR* data
175  essentially agree, lending confidence to the lab transition probabilities for the long wavelength lines.

176      Stellar spectroscopists usually focus on using the best available lab $gf$-values for abundance work.
177  But as the spectroscopic data sets attain ever-increasing resolution and signal-to-noise quality some
178  secondary atomic data considerations become important for the most accurate abundances. Odd-Z
179  elements and odd-*A* isotopes often yield transitions with significant hyperfine structure. Examples
180  of this have been well documented in recent Fe-peak studies ([17,23–25]. Less attention has been
181  paid to isotopic displacement of spectral lines of some elements. The isotopic wavelength offsets are
182  undetectably small in the *UV* and most of the optical spectral region, but they grow with increasing
183  wavelength.

184      Ni has five naturally-occurring isotopes, three of which have non-negligible percentages in
185  solar-system material: $^{58}$Ni, 68.1%; $^{60}$Ni, 26.2%; and $^{62}$Ni, 3.6%. For Ni I the presence of significant
186  isotopic splitting for several lines redward of 7000 Å has been demonstrated by [21]; see their
187  Figure 10. Hyperfine and isotopic subcomponents of spectral lines will always act to spread the
188  absorption in wavelength, desaturating the overall feature. Neglect of transition substructure can lead
189  to over-estimation of abundances, and for strong lines this can be a significant effect.

190      Examination of the solar photospheric spectrum [42] has called attention of the isotopic
191  substructure of Ti I transitions, which have been previously reported in laboratory studies (e.g.,
192  [43]). In solar-system material, Ti splits into these isotopes: $^{46}$Ti, 8.25%; $^{47}$Ti, 7.44%; $^{48}$Ti, 73.72%; $^{49}$Ti,
193  5.41%; and $^{50}$Ti, 5.18%. The isotopic broadening of optical Ti I lines is negligible, but detectable in
194  the near-*IR*. As an example, in Figure 5 we show one near-*IR* transition in the lab and in the solar
195  photosphere. Isotopic wavelength shifts are not resolved into individual components, but the extra
196  line broadening is evident. As with Ni, this effect can become important in deriving accurate elemental
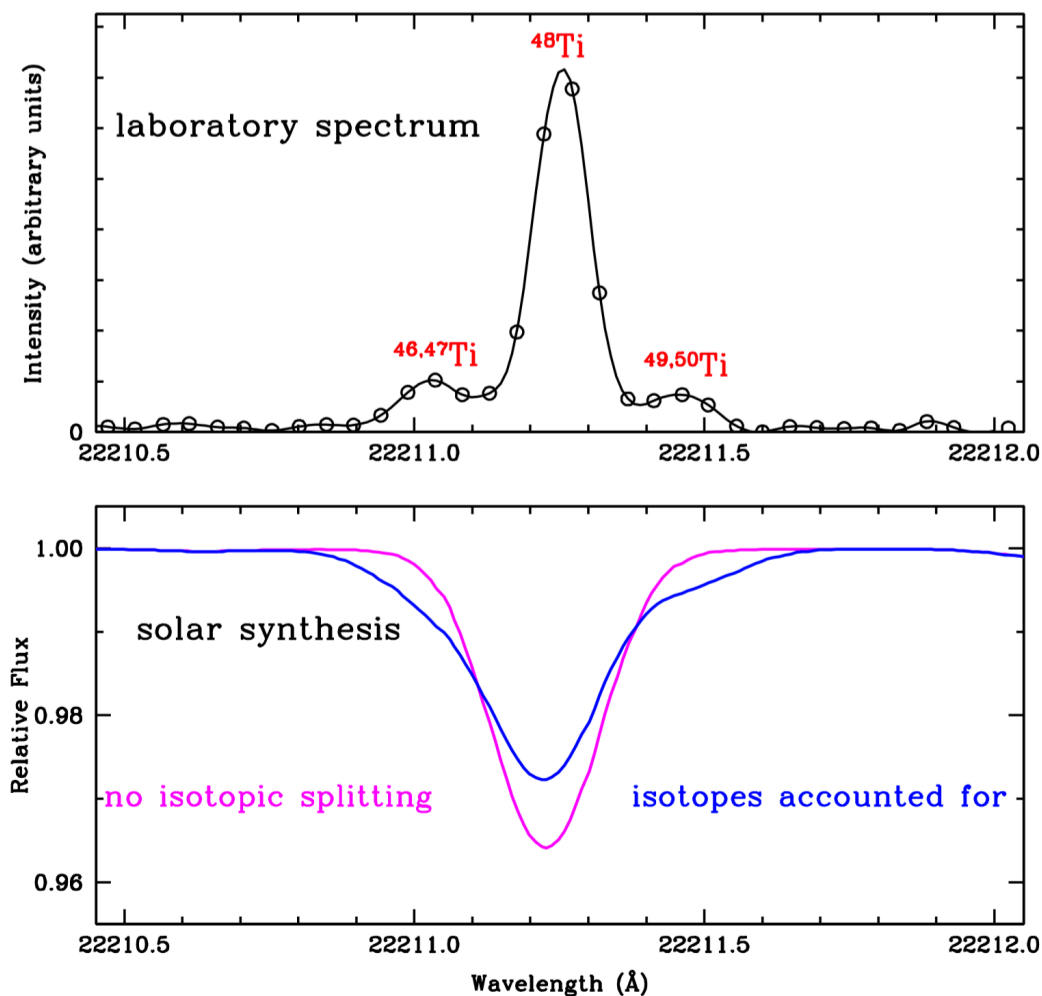197  abundances when Ti I lines become strong, as they surely will in cool red giant stellar spectra.

**Figure 5.** An example of isotopic broadening in Ti I transitions. In the top panel we show a laboratory emission spectrum of one of the near-*IR* lines; see [42] for details. In the bottom panel we show synthetic solar profiles for this transition with (blue) and without (magenta) proper accounting for the minor isotopes of Ti.

**Conflicts of Interest:** The authors declare no conflict of interest.

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