Accurate experimental log(gf)-values and their impact on the calculation of chemical abundances


Fourier Spectroscopy Laboratory – Imperial College London
OUTLINE

1. Why do we measure “log(gf)”?
2. What are “log(gf)”?
3. In the lab
1. Need for Laboratory Data

- The analysis of stellar spectra is vital in the determination of CHEMICAL ABUNDANCES.

- Large investment of TIME and MONEY to record spectra of astrophysical objects at unprecedented resolution, but LACK OF ACCURATE ATOMIC DATA!!!!

Earth-based laboratories needed to produce ACCURATE atomic data!!
Astronomy
(chemical abundances)

Experimental Spectroscopy
Atomic physics
Chemical abundances !!!!

Oscillator strength (f)

\[ \log(gf) = \log \left[ A_{ki} g_k \lambda_{ki}^2 \times 1.499 \times 10^{-14} \right] \]

Transition probabilities \((A_{ki})\)
Who are we?

Catania, 5 September 2017
2. Transition Probabilities

- Lifetime ($\tau_k$)
- Transition probability ($A_{ki}$)
  (Einstein coefficient for emission)

\[
\tau_k = \frac{1}{\sum_i A_{ki}}
\]
2. Intensity of a Line
2. Transition Probabilities

Thermodynamic equilibrium

\[ I_{ki} = \frac{1}{2} A_{ki} \frac{\hbar c}{\lambda_{ki}} N_k \]

Measure all transitions from a given upper energy level

\[ I_{ki} = M \frac{A_{ki} g_k \hbar c}{2\lambda_{ki}} \frac{N(T)}{Z(T)} e^{-\frac{E_k}{kT}} \]

\[ A_{ki} = \frac{BF_{ki}}{\tau_k} \]
Branching fractions

\[ BF_{ki} = \frac{I_{ki}}{\sum_i I_{ki}} = \sum_i A_{ki} \]

\[ \tau_k = \frac{1}{\sum_i A_{ki}} \]

\[ A_{ki} = \frac{BF_{ki}}{\tau_k} \]
2. Transition Probabilities

How can we get high quality transition probabilities?
3. In the lab

Atomic parameters

Atomic physics +

Plasma physics

Spectroscopy

ΔE = ħf

Catania, 5 September 2017
In the lab

a) GENERATE THE RADIATION (PLASMA)

b) ANALYSE THE RADIATION (SPECTRA)
In the lab...

What your research supposedly looks like:

- Data
- Data Acquisition
- Prototype
- Controller
- Computer

What your research actually looks like:

Figure 1. Experimental Diagram

Figure 2. Experimental Mess
Our lab!
a) The lamp
a) The lamp

- High voltage: ~600 V at 50-1000 mA
- Ne or Ne/Ar gas at 1-3 mbar
- Water cooled
- Attenuator: Glass
- Anode, Cathode, Anode
b) The spectrometer (FTS)
Spectra
1. Line identification

2. Intensity calibration

3. Correction of self-absorption

4. Fitting of the spectral lines
Experimental details

* **Spectral range**: 140 nm – 5 μm

* **Gas pressure**: 1-2 mbar

* **I lamp**: 300-1000 mA

* **Resolving power**: 2 000 000 (at 200 nm)
Importance of our high resolution
Importance of our high resolution
Hyperfine structure

Hyperfine split line at 8116.789 Å from the 21032 cm$^{-1}$ upper level
Isotopic effect

Isotopic Structure in $3d^74s^2 - 3d^8(3F)4p$ Ni II

SNR vs. Wavenumber (cm$^{-1}$)
The Critical Assessment of Atomic Oscillator Strengths

W. L. Wiese

National Institute of Standards and Technology, Gaithersburg, MD 20899, U.S.A.

Estimation of Inaccuracies in Oscillator Strength Calculations

A. Hibbert

Department of Applied Mathematics and Theoretical Physics, The Queen’s University of Belfast, Belfast BT7 1NN, N. Ireland
Critical aspects in an emission spectroscopy experiment:

- Measuring of all the transitions coming from an upper level
- Self-absorption
- Blends
- Spectral calibration
- Correct determination of the line intensity (fitting, SNR)
- ...
Critical factors when obtaining the intensity (area)

- Sufficiently separated lines
- Good signal-to-noise ratio
- Non self-absorbed lines
NIST Spectra Database

NIST Atomic Spectra Database Lines Data

Fe I: 1918 Lines of Data Found

Z = 26, Fe isoelectronic sequence

Wavelength range: 200 - 300 nm
Wavelength in: vacuum below 200 nm, air between 200 and 2000 nm, vacuum above 2000 nm
Highest relative intensity: 138000

Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

Primary data sources:
- Energy Levels: Nave et al. 1994
- Lines: Nave et al. 1994
- Transition Probabilities: Exner and Weese 2000

Query NIST Bibliographic Databases for Fe I:
- Energy Levels
- Line Wavelengths and Classification
- Transition Probabilities

Table:

<table>
<thead>
<tr>
<th>Observed Wavelength (nm)</th>
<th>Ritz Wavelength (nm)</th>
<th>Rel. Int. (?)</th>
<th>A_u (s^-1)</th>
<th>Acc.</th>
<th>E_i (cm^-1)</th>
<th>E_u (cm^-1)</th>
<th>Lower Level Cont., Term, J</th>
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<th>Type</th>
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NIST uncertainties

The uncertainties are obtained from critical assessments, and in general, reflect estimates of predominately systematic effects discussed in the NIST critical compilations, cited in the bibliography.

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<td>E</td>
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Publications on Atomic Transition Probabilities that include numerical data

Spectrum included: Fe I

233 references found

Go to main Transition Probabilities Bibliography search form

The output below may contain links to sites outside of NIST because they have information that may be of interest to our users. NIST does not necessarily endorse the views expressed or the facts presented on these sites. Further, NIST does not endorse any commercial products that may be advertised or available on these sites.

New Fe I level energies and line identifications from stellar spectra. II. Initial results from new ultraviolet spectra of metal-poor stars,
R. C. Peterson, R. L. Kurucz, and T. R. Ayres,
DOI:10.3847/1538-4357/aa6253

Spectral properties of cool stars: Extended abundance analysis of 1,617 planet-search stars,
J. M. Brewer, D. A. Fischer, J. A. Valenti, and N. Piskunov,
DOI:10.3847/0067-0049/225/3/32

New Fe I level energies and line identifications from stellar spectra,
R. C. Peterson and R. L. Kurucz,
DOI:10.1088/0067-0049/216/1/1

Fe I oscillator strengths for the Gaia-ESO survey,
DOI:10.1093/mnras/stu780

Fe I oscillator strengths for transitions from high-lying even-parity levels,
DOI:10.1088/0067-0049/215/2/23
Our results

Table 4. Experimental BF\textsuperscript{a}s, transition probabilities and log\((gf)\) values for 16 odd-parity energy levels of Fe I.

<table>
<thead>
<tr>
<th>Wavelength\textsuperscript{a} (nm)</th>
<th>Upper Level\textsuperscript{a}</th>
<th>Lower Level\textsuperscript{a}</th>
<th>BF\textsuperscript{b}</th>
<th>(U_{BF}\textsuperscript{b}) (%)</th>
<th>(A_{ul}\textsuperscript{c}) (10\textsuperscript{6} s\textsuperscript{-1})</th>
<th>This experiment\textsuperscript{d}</th>
<th>Published\textsuperscript{e}</th>
<th>Ref.</th>
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<td>1.0000</td>
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<td>108.70 (5)</td>
<td>0.43 ± 0.02</td>
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<td>463.0120</td>
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<td>18378.185</td>
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<td>0.12 (13)</td>
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<td>2.49 (6)</td>
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<td>7985.784</td>
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<td>0.0049</td>
<td>7.5</td>
<td>1.90 (9)</td>
<td>-1.71 ± 0.04</td>
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<td>0.1794</td>
<td>5.2</td>
<td>69.00 (7)</td>
<td>-0.34 ± 0.03</td>
</tr>
</tbody>
</table>
Our work now

- New measured transition Probabilities of Sc II (Lund, Sweden)
- New transition probabilities of Fe I coming soon

New data needed?!
Special session:

“Atomic and molecular data needs for astronomy and astrophysics”
THANK YOU FOR YOUR ATTENTION!
2. Thinking about “waves”
2. Joseph Fourier

“Any function of a variable, whether continuous or discontinuous, can be expanded in a series of sines of multiples of the variable.”

* Some discontinuous functions are the sum of infinite series!

*The Analytic Theory of Heat*

(1822)
2. Fourier analysis

“Fourier analysis is not often of direct use in studying light waves because it is impossible to observe directly the form of a light wave”

* Optical frequencies $\rightarrow 10^{-15}$ s (too fast)
* Our detector measures up to $10^{-9}$ s
2. Albert A. Michelson
“The envelope of the interferogram has exactly the same shape as that of the original wave, but the carrier frequencies are reduced by the factor $v/c$.”
In the lab...
\[
\log(g_l f) = \log \left[ A_{ul} g_u \lambda^2 \times 1.499 \times 10^{-14} \right]
\]

\[
BF_{ul} = \frac{I_{ul}}{\sum_l I_{ul}} = \frac{A_{ul}}{\sum_l A_{ul}}
\]

\[
\tau_u = \frac{1}{\sum_l A_{ul}}
\]
\[ A_{ul} = \frac{BF_{ul}}{\tau_u} \]

\[
\left( \frac{\Delta BF_{ul}}{BF_{ul}} \right)^2 = (1 - 2BF_{ul}) \left( \frac{\Delta I_{ul}}{I_{ul}} \right)^2 + \sum_{j=1}^{n} BF_{uj}^2 \left( \frac{\Delta I_{uj}}{I_{uj}} \right)^2
\]

\[
\left( \frac{\Delta A_{ul}}{A_{ul}} \right)^2 = \left( \frac{\Delta BF_{ul}}{BF_{ul}} \right)^2 + \left( \frac{\Delta \tau_{ul}}{\tau_{ul}} \right)^2
\]