

# Oscillator strengths and their uncertainties: A tale of caution for non-LTE analysis

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# Contents

- I. Motivation
- II. Basics of oscillator strengths ( $f$ -values)
- III. Experimental  $f$ -values
- IV. Theoretical  $f$ -values
- V. Manipulating  $f$ -values for line structure
- VI. Uncertain(ties) comments

# I. Motivation

for assessing errors

“... a vital part of the determination of an oscillator strength is the assessment of a probable error. If this is not done reliably, for example, an apparent detection of non-LTE in a stellar atmosphere might only be due to errors in the adopted oscillator strengths.”

D.E. Blackwell (1990) (ASOS3 proceedings)

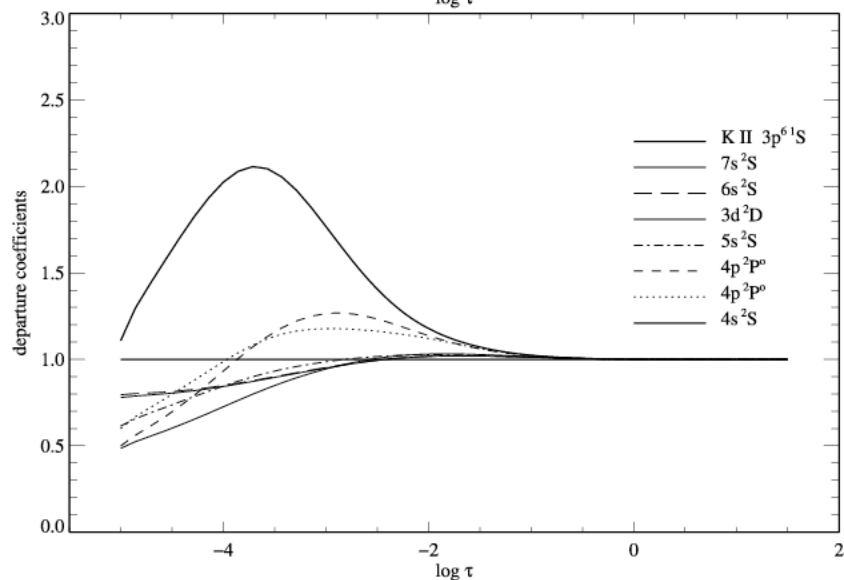
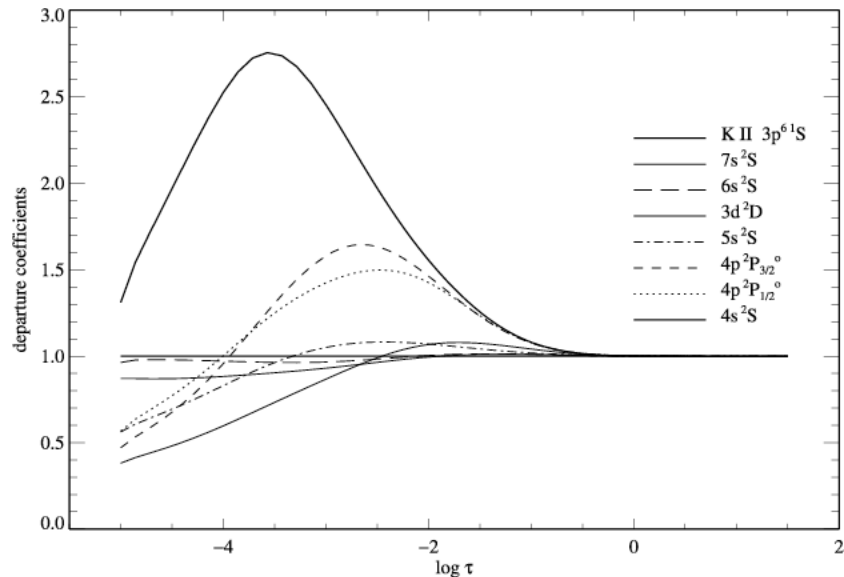
for further laboratory work

“Lines from different energy levels can be used to determine the iron abundance of a star and test the assumptions about thermal equilibrium. This is a direct use of the data which we plan to produce within the FERRUM project.”

Z.S. Li et al. (1999, Eur. Phys. J. D 6, 9)

**Comments are from physicists – not astronomers!**

# Consider “ $b_n$ versus $\sigma f$ ”



Equiv. width of a line:  $W = n_1 g_1 f_{12}$

LTE  $W_{lte} = (ngf)_{lte}$

non-LTE  $W_{non} = (ngf)_{non}$

Comparing analyses:

$W_{non} = W_{lte}; (ngf)_{non} = (ngf)_{lte}$

$n_{non}/n_{lte} = f_{lte}/f_{non}$

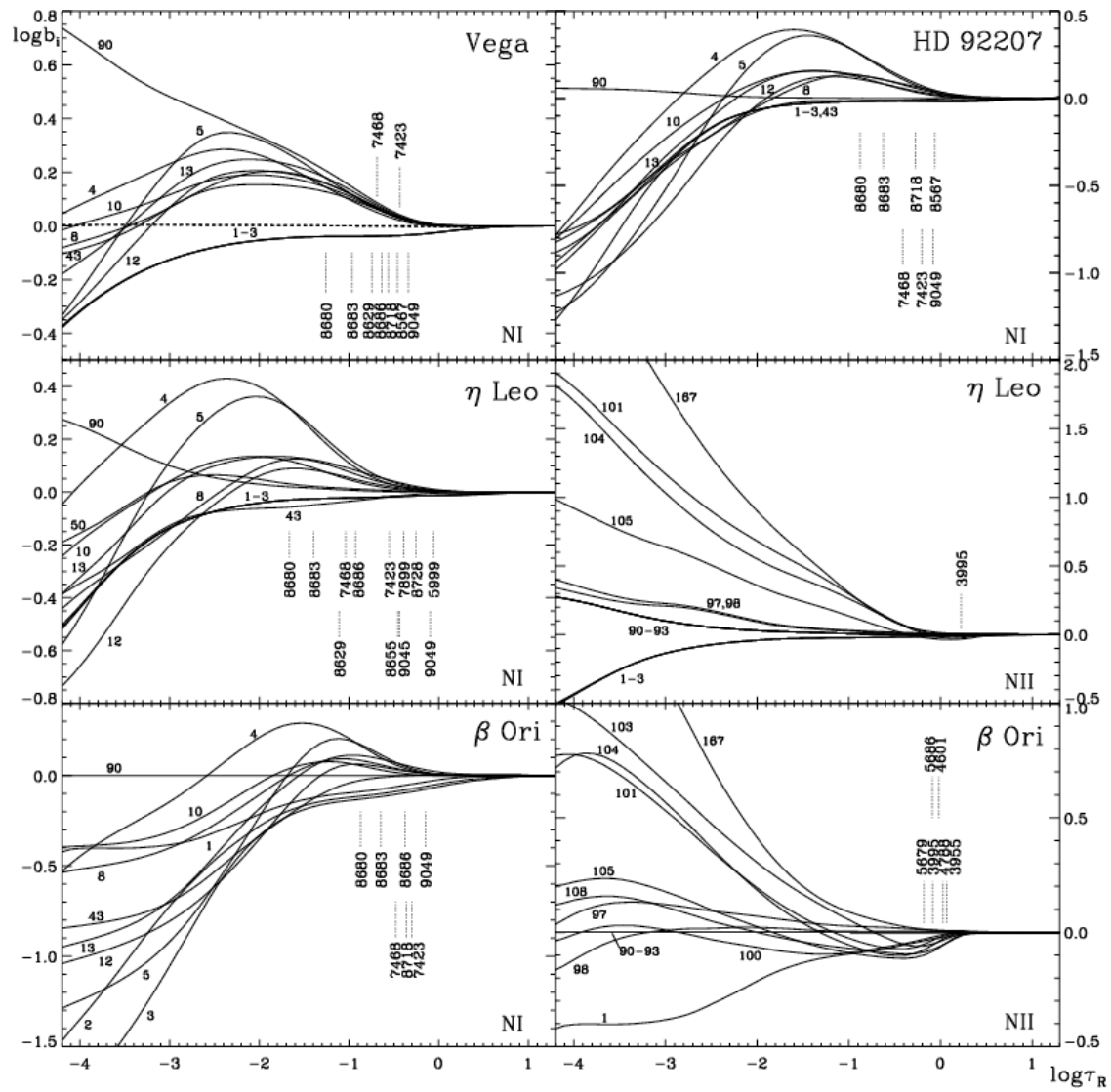
$b_n = n_{non}/n_{lte} = f_{lte}/f_{non}$

Where are lines formed ( $\tau$ )?

Which levels are involved?

What is the uncertainty in  $f$ ?

What uncertainty can you accept ?



Przybilla & Butler, 2001, A&A 379, 955, “Non-LTE line formation for N I/II:...”

## II. Basics of oscillator strengths, $f$

What is  $f$ ?

$f$  originates from the classical approach to the absorption of radiation and is related to the real part of the index of refraction and the absorption coefficient.

The number of classical oscillators per atom for a particular transition,  $\eta = n_i f_i$

where,  $\eta = \#$  density of equivalent classical oscillators

$n_i = \#$  density of atoms in upper (or lower) level

$f =$  is dimensionless and related to  $A$

$$f_{12} = (g_2/g_1) (\epsilon_0 m_e c^2)/(2\pi e^2 \nu^2) A_{21}$$

$A_{21}$  is the spontaneous decay rate

(cont.)

- $f$  is also thought of as the fraction of valence electrons likely to participate in the transition of interest
  - $f$  is one measure of line strength, often weighted (multiplied) by the statistical weight of the level
  - $gf$  values become larger when a) there are fewer decay channels, and b) the number of sublevels ( $g_J = 2J + 1$ ) increases
- \* transitions with large  $gf$  values do not necessarily lead to strong observable spectral lines. Both the Boltzmann factor ( $e^{-E/kT}$ ) and the total abundance are considerations.

## Relationships between $f$ , $A$ , $\kappa$ , ...

For two level atom we have Einstein coefficients  $A_{21}$ ,  $B_{12}$ ,  $B_{21}$

$$A_{21} = [8\pi h \nu^3 / c^3] B_{21} \quad ; \quad B_{21}/B_{12} = g_1/g_2$$

Therefore, if we can measure  $A_{21}$ , we can determine  $B_{12}$  &  $B_{21}$

Can include the effect of collisions in the two-level atom,  $C_{ij}$

$B_{12}$  is related to absorption coefficient,  $\kappa(\nu)$

$$dB_{12}/d\nu = (c/n_1 h \nu_0) \kappa(\nu)$$

And  $\kappa(\nu)$  is related to optical depth ( $\tau$ ) and the line profile ( $I/I_0$ ):

line absorption coeff.,  $l_n = (N/\rho) \alpha(\nu) = (N/\rho) \times (\text{constants}) \times f \times V(u,a)$



## $f$ -values: miscellaneous

\* Natural line broadening:  $dv_{ij} = (2\pi\tau_i)^{-1} + (2\pi\tau_j)^{-1}$

Most natural line broadening coefficients is computed as independent of lifetime. Synthetic spectrum modeling shows that better line profile fits may be obtained by using lifetime dependent line broadening.

\* Normalization of the atomic absorption coefficient,  $\alpha(\nu) = (\pi e^2/m_e c) f$

\*  $f$  sum rules: the Tomas-Kuhn-Reich sum rule

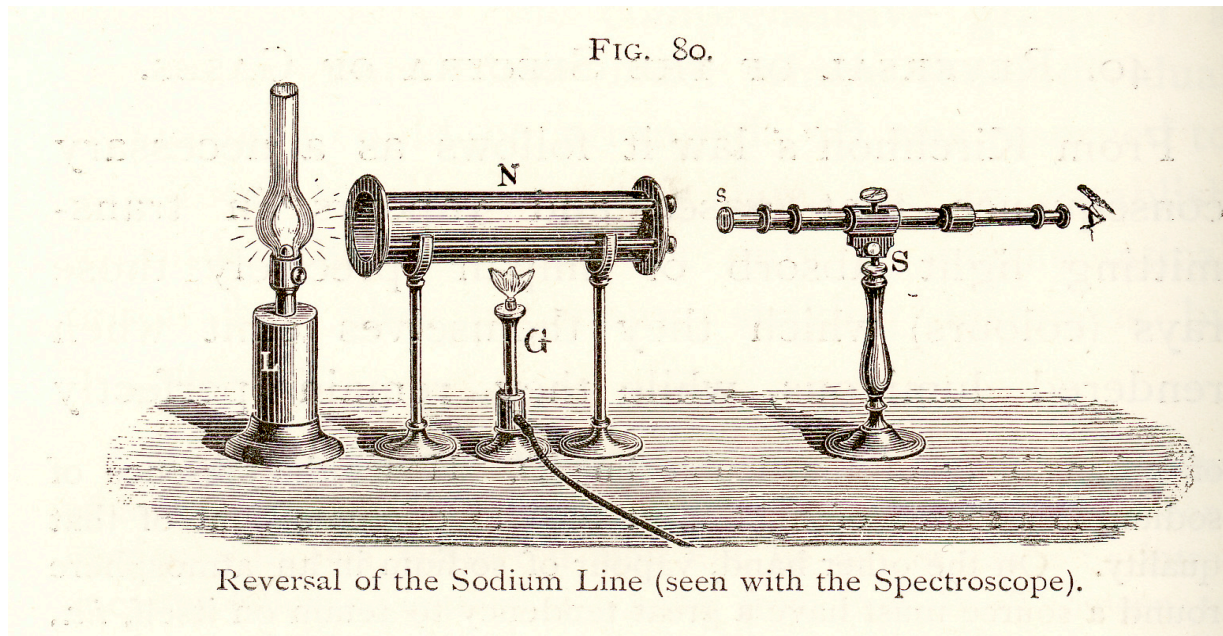
$$\sum f_{iu} - \sum (g_l/g_i) f_{li} + f_{il} d\varepsilon = z, \text{ number of electrons}$$

where,  $i$  = level starting from,  $l$  = index for lower energy levels

$u$  = index for upper energy levels,  $\varepsilon$  = energy in continuum

\* In general,  $f_{ij} = - (g_j/g_i) f_{ji}$

### III. Experimental oscillator strengths



Why measure  $A$  or  $f$  ?

(Because we can!)

Provides basic data: lifetime ( $\tau$ ),  $A$ -value,  $f$ -value, [line strength ( $S$ )]

Allows for tests of atomic structure theory:

non-relativistic Hartree-Fock

relativistic corrections

fully relativistic, multi-configuration Dirac-Fock (MCDHF)

=> Lead to a *fundamental* knowledge of atomic structure

Older techniques used for determining  $f$ -values include use of:

*Furnace* (1m carbon tube heated to 3000K by high current, absorption technique, thermal excitation, limited to low excitation (3 eV))

*Shock tube* (absorption or emission)(LTE over wide temp. & density range including 'stellar' plasma of 3000-9000K,  $10^{20}$  cm<sup>-3</sup>, but requires measurement of temp. and density for analysis.)

Conversion of emission line intensities (Corliss & Bozman 1962)

*Beam-foil* (a couple of facilities still functioning)

Present day techniques for lifetime measurements include:

*Beam-laser*

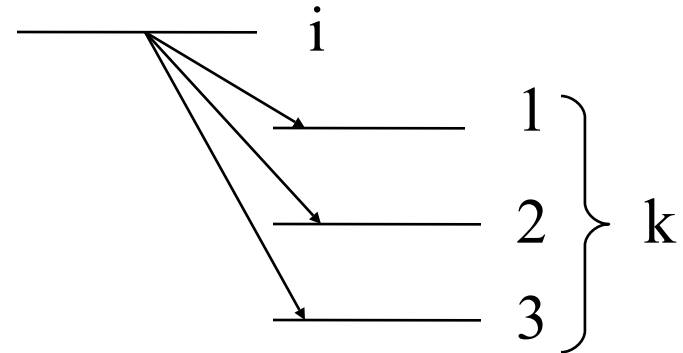
*Laser-laser (LIF)*

*Laser probing* in storage rings (forbidden transitions)

## Components of the Experimental Oscillator Strength

Line intensity,  $I_{ik} = N_i g_i A_{ik}$

Branching fraction,



$$(\text{BF})_{ik} = A_{ik} / \sum_k A_{ik} = I_{ik} / \sum_k I_{ik}$$

Level (mean) lifetime,  $\tau_i = (\sum_k A_{ik})^{-1}$

Transition probability,  $A_{ik} = (\text{BF})_{ik} / \tau_i$  [ $\lambda$  (nm),  $A$  ( $\text{s}^{-1}$ )]

Oscillator strength,  $f = 1.499 \times 10^{-14} (g_i / g_k) \lambda^2 A_{ik}$

\* Measuring  $\tau$  and  $I$  yields  $f \Rightarrow$  1 or 2 experiments

The methodology applies to emission line spectroscopy where the lifetime of the upper level is known.

Wavelength coverage must be extensive to record all lines in multiplet to reduce the missing intensity ('residual').

S/N must be high enough to measure all lines in multiplet.

Light source need not be LTE in nature (for example, hollow cathode)

Must have sufficient excitation to populate the upper level of the transitions.

Excitation influenced by carrier gas:

Argon - heaviest atom, can reach 10eV

Neon - can reach 15 eV

Helium – lightest atoms, fastest speed, highest excitation possible, but ...

## Oscillator strengths for lines of Se I (VALD)

| Elm Ion | WL(A)     | log(gf) | Exc. lo | J lo | Exc. up | J up | Labels       | Ref  |
|---------|-----------|---------|---------|------|---------|------|--------------|------|
| Se 1    | 1960.9020 | -0.230  | 0.0000  | 2.0  | 6.3230  | 1.0  | 4p4 3P 5s 3S | CB   |
| Se 1    | 2039.8510 | -0.110  | 0.2470  | 1.0  | 6.3230  | 1.0  | 4p4 3P 5s 3S | CB   |
| Se 1    | 2062.7880 | -0.520  | 0.3140  | 0.0  | 6.3230  | 1.0  | 4p4 3P 5s 3S | CB   |
| Se 1    | 2074.7940 | -1.440  | 0.0000  | 2.0  | 5.9740  | 2.0  | 4p4 3P 5s 5S | CB   |
| Se 1    | 2164.1650 | -1.000  | 0.2470  | 1.0  | 5.9740  | 2.0  | 4p4 3P 5s 5S | MULT |
| Se 1    | 8918.8030 | 1.290   | 5.9740  | 2.0  | 7.3640  | 3.0  | 5s 5S 5p 5P  | CB   |
| Se 1    | 9001.8980 | 0.000   | 5.9740  | 2.0  | 7.3510  | 2.0  | 5s 5S 5p 5P  | GUES |
| Se 1    | 9038.5460 | 0.000   | 5.9740  | 2.0  | 7.3450  | 1.0  | 5s 5S 5p 5P  | GUES |

References: 1. Bell heavy: Ga to Ba

## Experimental $A$ values for Se I

Lifetime measurements ( $\tau$ ):

Bengtsson et al. (1992, Z. Phys. D 23, 29)  $\tau(5s\ ^3S^o_1, 50996.03\text{ cm}^{-1}) = 2.9(5)\text{ ns } (+/-\ 17\%)$

Bengtsson et al. (1992, J. Phys. II France 2, 773)  $\tau(5s\ ^5S^o_2, 48182.19\text{ cm}^{-1}) = 493(15)\text{ ns } (+/-\ 3\%)$

Dynefors (1975, Physica Scripta 11, 375)

Line intensities:

Ubelis & Berzinsh (1986, Physica Scripta 34, 805)

$I_{196.1} : I_{204.0} : I_{206.3} = (100 +/- 1) : (44 +/- 1) : (15 +/- 0.5)$  **(1 – 5 % uncertainties)**

$I_{207.5} : I_{216.4} = (100 +/- 5) : (18 +/- 1)$

Comparison of transition probabilities:

|                              | $A(196.1)$ | $A(204.0)$ | $A(206.3)$   |            |
|------------------------------|------------|------------|--------------|------------|
| (Ubelis&Berzinsh)+(Bengtson) | 100        | 46         | 15           | experiment |
| Ubelis & Berzinsh (1986)     | 100 +/- 1  | 44 +/- 1   | 15.5 +/- 0.5 | experiment |
| Gruzdev (1969)               | 100        | 48         | 16           | theory     |
| Garpman et al. (1974)        | 100        | 50         | 17           | theory     |
| Lavrence (1967)              | 100        | 47         | 16           | theory     |
| Knox & Olechna (1967)        | 100        | 34         | 3.8          | theory     |
| Corliss & Bozman (1962)      | 100        | 130        | 48           | experiment |
| Krempl & Schmid (1968)       | 100        | 238        | 240          | experiment |



# Experimental Oscillator Strength, Se I $\lambda$ 1960.902Å

Line intensity,  $I_{12} = N_1 g_1 A_{12}$

Branching fraction,

$$(BF)_{12} = I_{12} / \sum_k I_{1k} = 100 / (100 + 44 + 15) = 0.629$$

Transition probability,  $A_{12} = (BF)_{12} / \tau(^3S_1)$

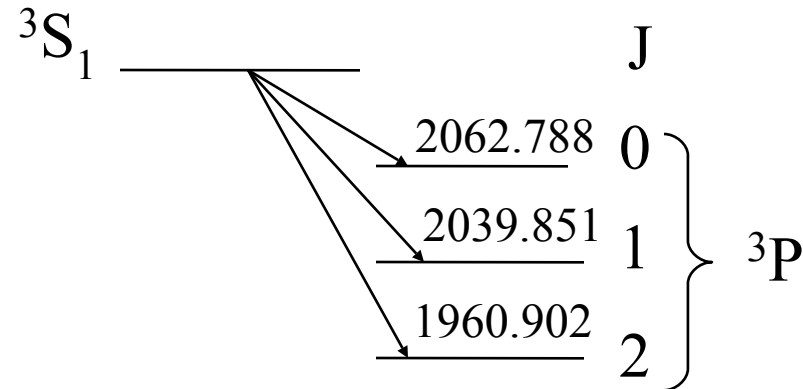
$$= 0.629 / (2.9 \times 10^{-9}) = 2.169 \times 10^8 \text{ s}^{-1}$$

Oscillator strength,

$$(gf)_{12} = 1.499 \times 10^{-14} g_1 \lambda^2 A_{12} \quad [\lambda \text{ (nm)}, A \text{ (s}^{-1})]$$

$$= 1.499 \times 10^{-14} (3) \lambda^2 (2.169 \times 10^8) = 0.375$$

$$\log (gf) = -0.426$$



## Comparison of oscillator strengths for Se I

| Wavelength<br>$\lambda(\text{\AA})$ | log $gf$ |        | comments       |
|-------------------------------------|----------|--------|----------------|
|                                     | CB       | UB + B |                |
| 1960.902                            | -0.230   | -0.426 | resonance line |
| 2039.851                            | -0.110   | -0.747 |                |
| 2062.788                            | -0.5     | -1.208 |                |
| 2074.794                            | -1.440   | -2.255 | resonance line |
| 2164.165                            | -1.000   | -2.963 |                |

CB = Corliss & Bozman (1962)

UB = Ubelis & Berzinsh (1986)

B = Bengtsson et al. (1992a,b)

*Why are the CB values still found in databases?*

The work of C.H. Corliss & W.R. Bozman: Importance and Limitations  
“Experimental Transition Probabilities for Spectral Lines of Seventy Elements”  
NBS monograph 53, (1962)

**Originally intended** to determine relative intensities of spectral lines for quantitative spectroscopic analysis, but realized that useful  $f$ -values could be derived from the measurements.

Data: 2000 -9000 Å, arc spectra photographed in 5 settings  
electrodes used a 1:10000 ratio of element:Cu

Procedure to determine  $f$ -values:

- measure line intensities,  $I$
- determine (arc) source  $T_{\text{eff}}$  from intensities and *published*  $A$  for many elements  
(Boltzman eq.) ( mean  $T_{\text{eff}}$ )
- measure degree of ionization for many elements from  $I$  and *published*  $A$ , then mean value for electron density, and the degree of ionization for all elements
- determine relative transition probabilities on a uniform scale for all classified lines
- place uniform scale on a normalized absolute scale by comparison with *published* absolute  $A$  values

Result:  $f$ -values for 25000 lines over 70 elements, an incredibly useful resource

However, it was eventually realized that CB *gf* values may have large and systematic errors.

“As a result of the two shock tube absorption experiments we recognized that the 'normalization function' applied by Corliss and Bozeman in the free-burning arc for high excitation lines was incorrect, making their *gf*-values nearly on order of magnitude too high.”

W.M. Parkinson (circa 1970), regarding Fe I

\* [Add historical comments on solar abundances and *f*-values in the 1960s]

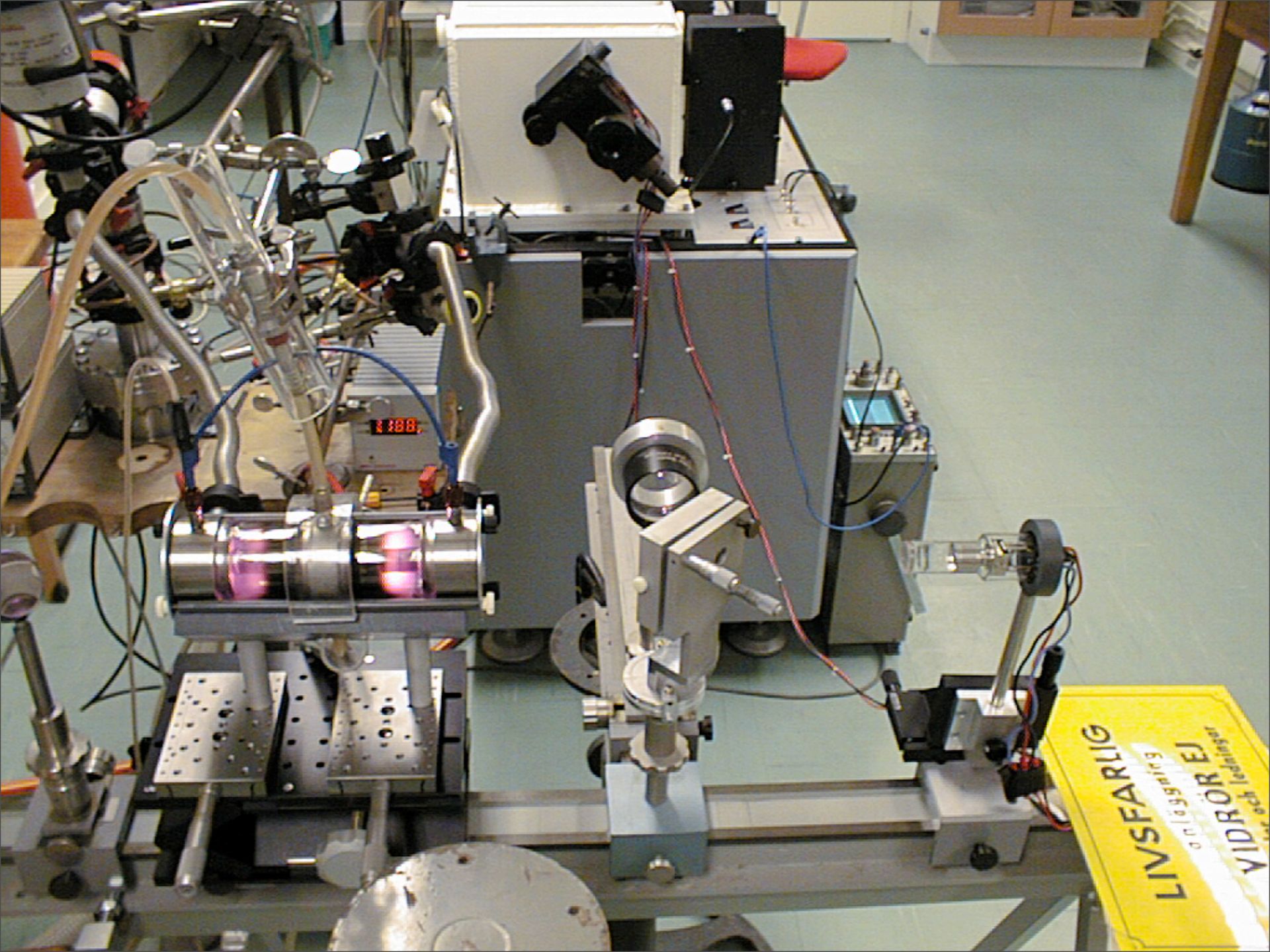
Updating the work of CB:

In his line list R. Kurucz has:

- a) included work of CB or MC directly
- b) made systematic ion-dependent corrections,  $MC' = MC + x.xx$

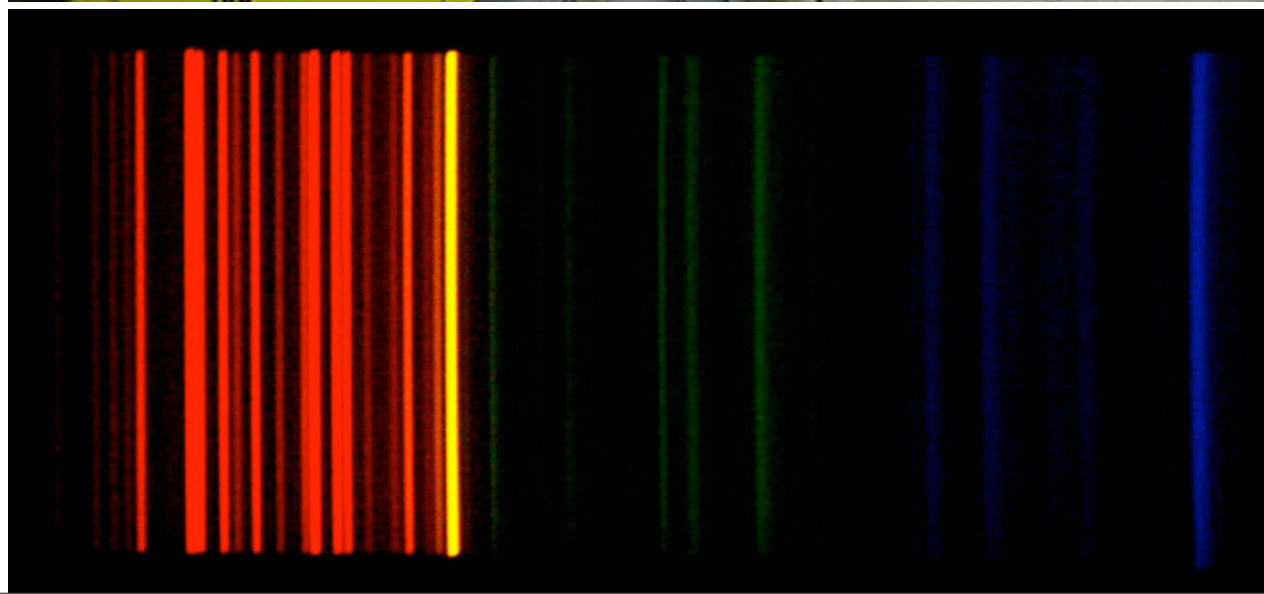
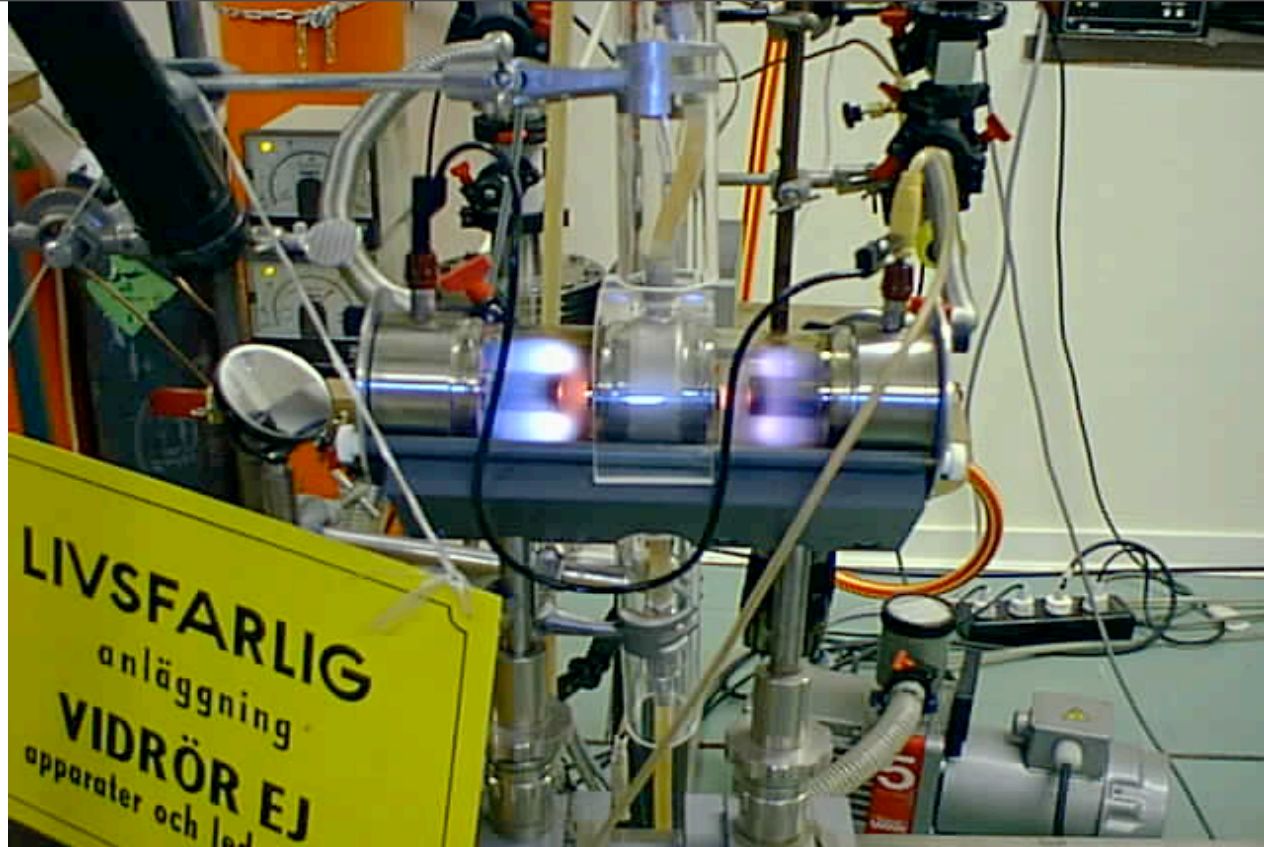
Laboratory Astrophysics:  
Daytime observing runs





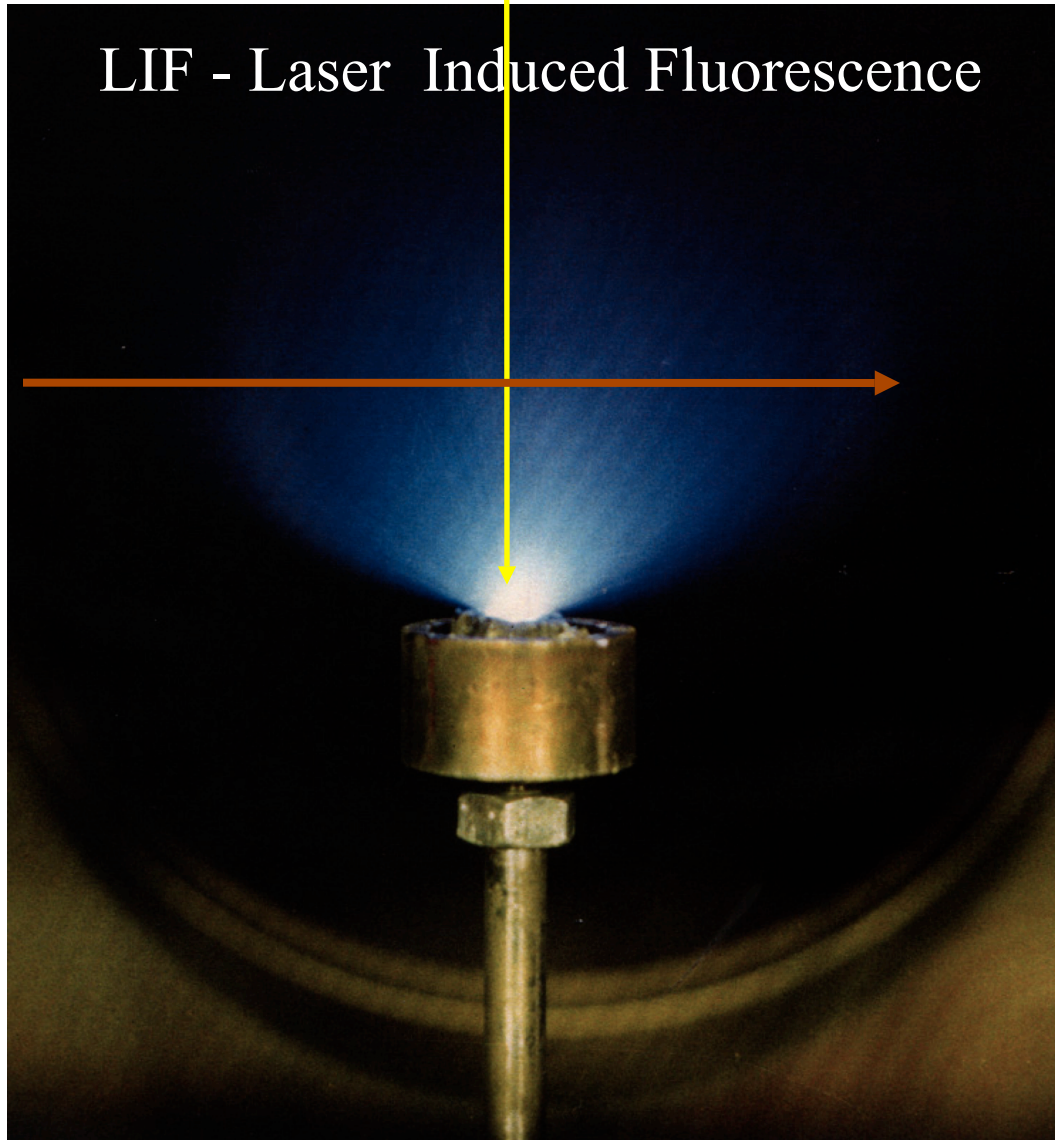
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anläggning  
VIDRÖR EJ  
och ledningar



# Atomic lifetime measurements

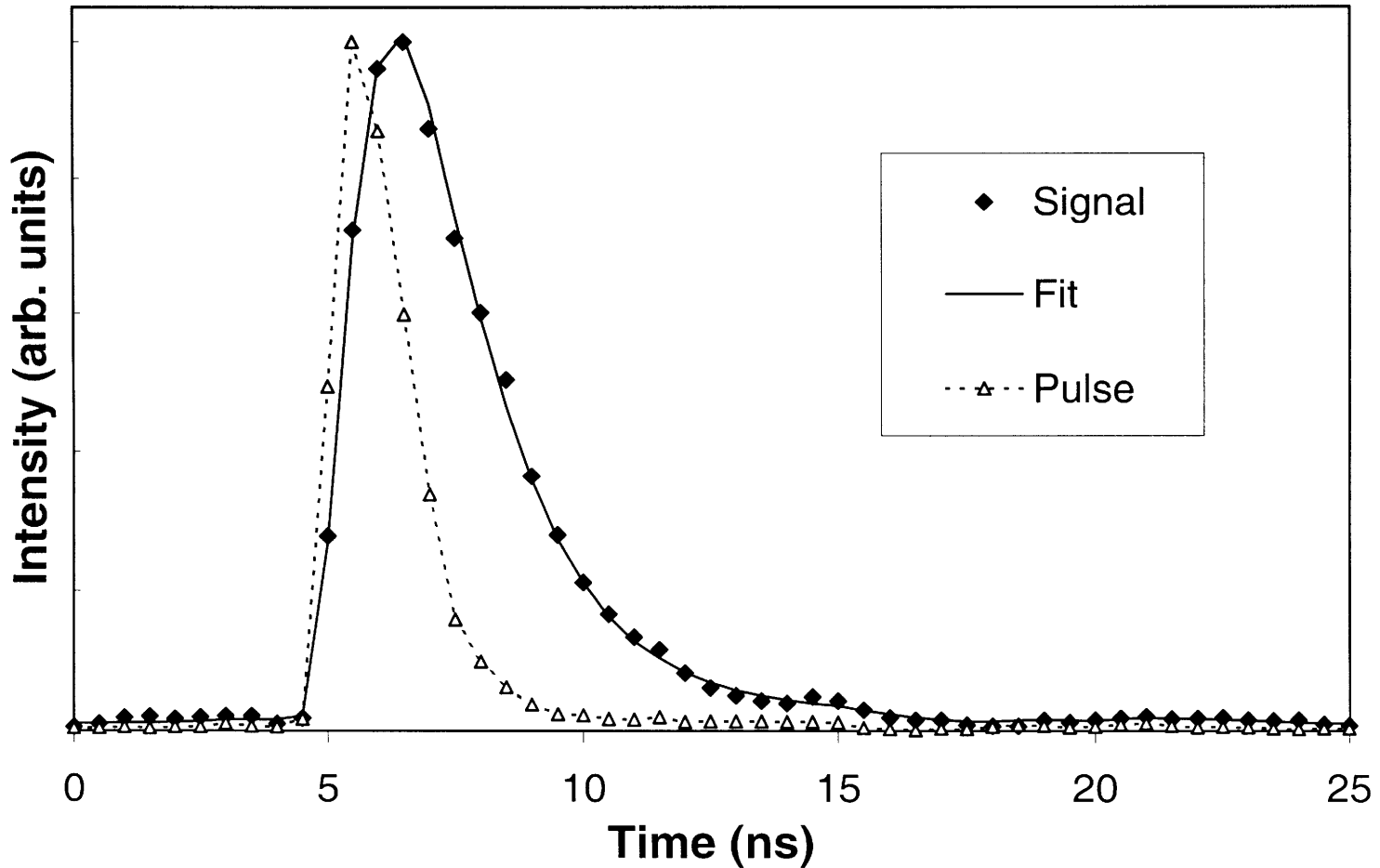
LIF - Laser Induced Fluorescence





Fluorescence decay curve for Ce III  $4f( {}^2F^0 ) 6p(5/2,3/2)$

Mean lifetime,  $\tau$ , determined from an exponential fit to curve.



# Laser Induced Florescence (LIF)

Double-laser system to create a plasma cone and populate excited states

Pros:

**Selective excitation process** (narrow bandwidth)

Can measure line intensity with same experiment, but with lower accuracy than spectroscopy

Cons:

Limited lifetime range due to experiment set-up, 1 – 100 ns (in Lund), allowed states only

Limited ion range (first three spectra)

Excitation conditions limited by the dyes

Time consuming process, need to measure levels individually

## Related techniques:

Beam-laser

Laser-laser

Storage rings with laser excitation: forbidden transitions

# Measurement of $\tau$ by Beam-Foil Spectroscopy

Pioneered in the 1960s: Provided much needed data.

Kay 1963, Phys Rev Letters 5, 36; Bashkin 1964, Nucl.Inst.Meth., 258

Saved in the mid-1970s

ANDC correction (Arbitrary Normalization Decay Curve), Curtis, L.J. et al.

Outdated by the 1990s

a couple of facilities still exist (Toledo, RIKEN)

Pros:

Any charge state, any element

Large lifetime range can be measured, 1 ps – 100 ns

High chemical purity, can observe one element

Cons:

Non-selective excitation, leading to cascade effects

Doppler effects

In practice, limited to lowest excitation states.

## Uncertainty regimes

Published (experimental and theoretical) uncertainties by NBS/NIST follow guidelines established decades ago:

(AA < 1%), A < 3%, B < 10%, C < 25%, D < 50%, E > 50%

Most measured lines have accuracy no better than C.

Theoretical *gf*-values tend to be labeled E.

## IV. Theoretical $f$ -values – the ultimate prize

The practical motivation for theoretical  $f$ -values is resources. Experiment will not be able to produce a large number of  $f$ -values.

Different theoretical formalisms (potentials, for example)

Dirac, Dirac-Fock, Hartree-Fock, Breit-Pauli, MCDHF, ...

non-relativistic (Breit-Pauli) vs relativistic (Dirac-Fock) vs. in-between  
core-core, core-valence, valence-valence electron interactions

Different codes and people for same formalism

## The approach to theoretical $f$ -values

$S$  (line strength)  $\rightarrow A$  (transition rate)  $\rightarrow f$  (oscillator strength)

1) Wavefunctions are determined and transition energy is computed.

**TEST:** compare energies with observations (not necessarily done here)

2)  $S(\gamma_i J_i, \gamma_k J_k) = \langle \Psi(\gamma_i J_i) \| O^k \| \Psi(\gamma_k J_k) \rangle^2$        $O^k$ , length (r) or velocity (E)  
operator

3)  $A(\gamma_k J_k, \gamma_j J_j) = (4/3) [\alpha \Delta E_{ik}]^3 S(\gamma_i J_i, \gamma_k J_k) / g_{Jk}$

4)  $f(\gamma_i J_i, \gamma_k J_k) = (2/3) \Delta E_{ik} S(\gamma_i J_i, \gamma_k J_k) / g_{Ji}$

Compare with typical formulas linking  $A$ ,  $f$ ,  $S$

$$A_{ki} = 6.6703 \times 10^{15} g_i f_{ik} / (g_k \lambda^2) = 2.0261 \times 10^{18} S / (g_k \lambda^3)$$

# Testing theoretical transition data

## Line strength S

Length form is independent of the energy; ( $S_L$ ) and is more stable to adding new effects

Velocity form = ( ... ) /  $\Delta E_{ik}$ ; ( $S_V$ )

$S_L = S_V$  for exact  $\Psi$

For approximate  $\Psi$  agreement is necessary but not sufficient

1) Transition energies,  $\Delta E$ , are used as test of *ab initio* calculations

Not appropriate for semi-empirical calculations (Cowan code, for example), where the energies are fixed as input.

2) The agreement between length and velocity *f*-values is a second test

Good test for LS, non-relativistic

Velocity in relativistic theory is difficult to work with

Transition dependent

*Theoreticians do not think of uncertainties in the same way as experimentalists.*

## V. Manipulating $f$ -values for line structure

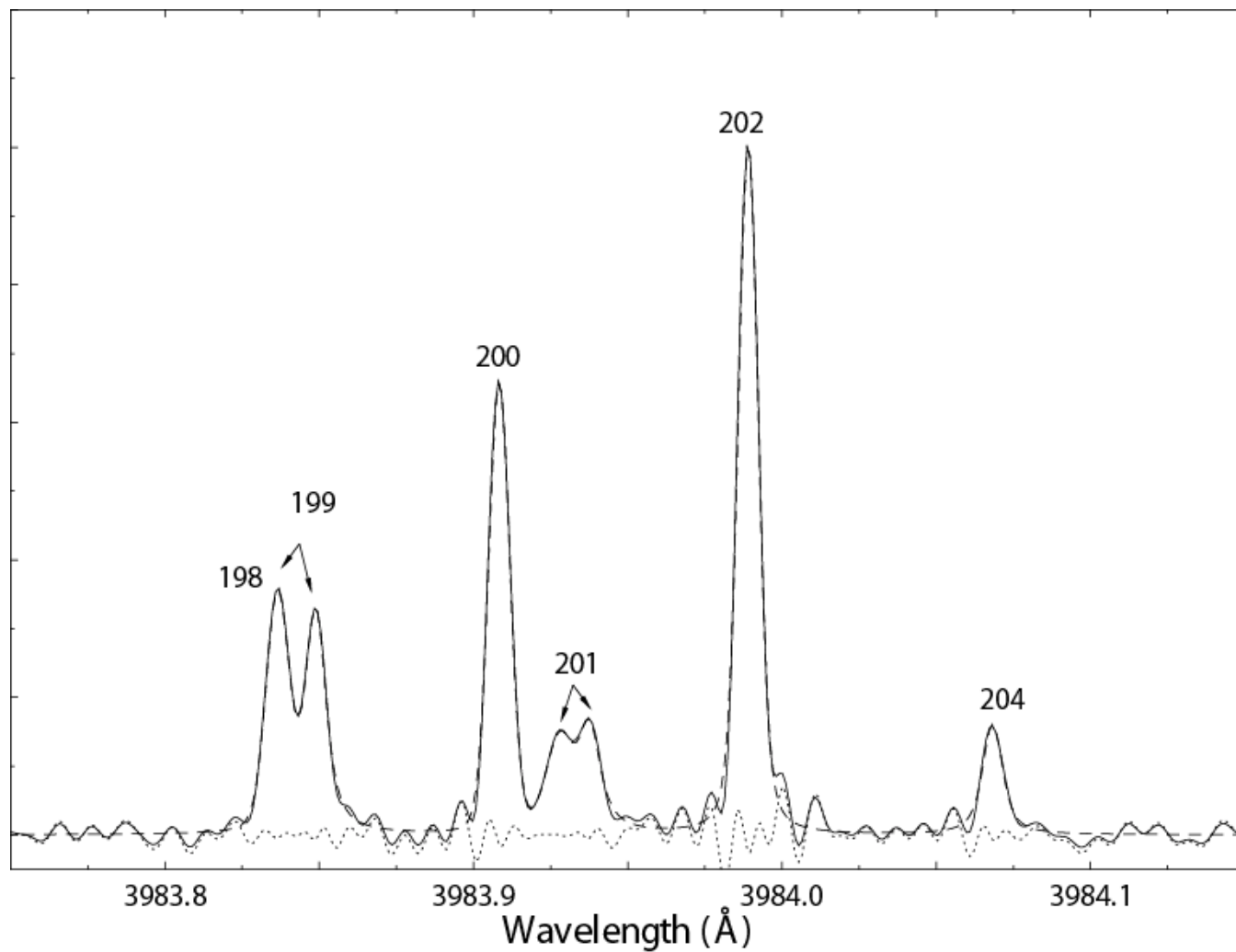
Isotope structure – the influence of nuclear mass and charge distribution on the shifting of atomic energy levels. (IS – isotope shift)

Hyperfine structure (hfs) – the interaction of the electric fields of the nucleus and electron shifts the atomic energy levels

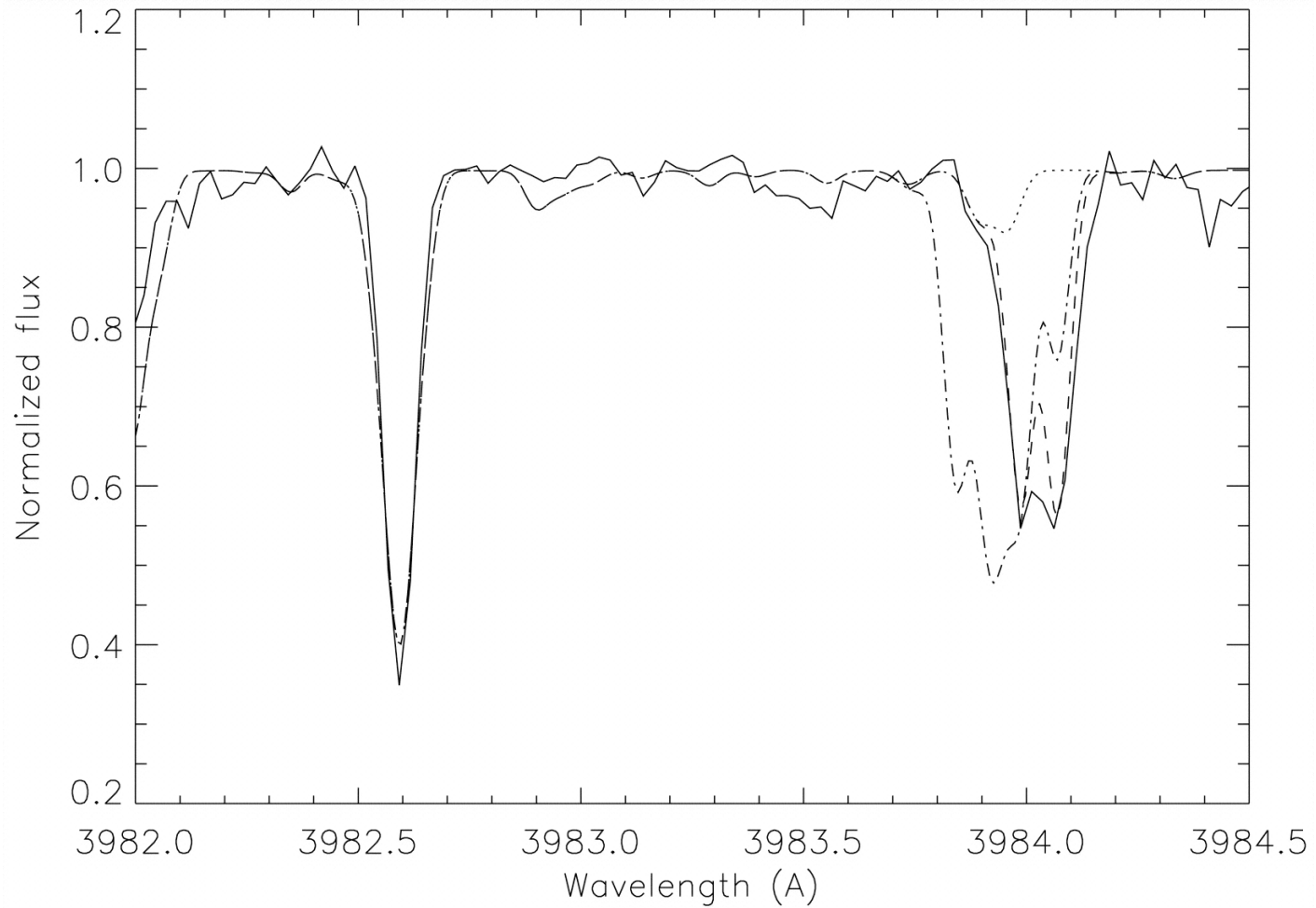
These two effects are often acting simultaneously in a transition.



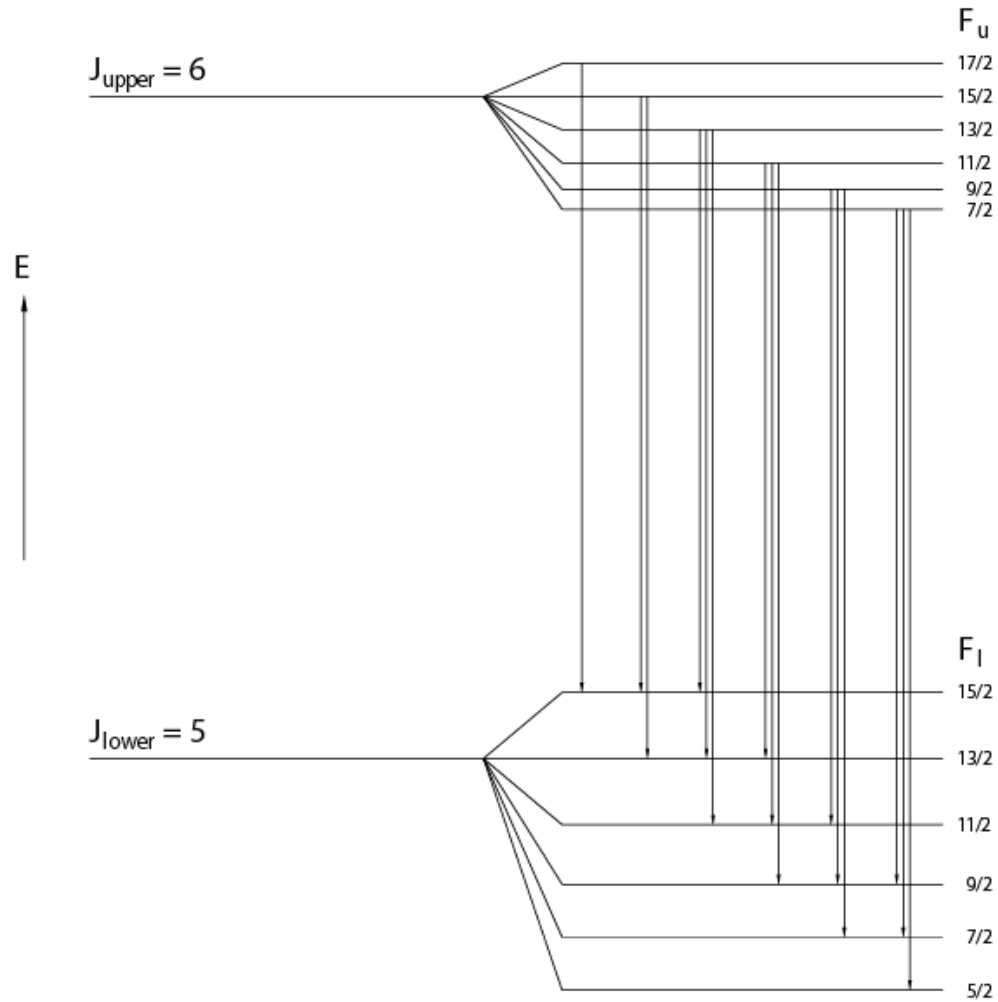
# Laboratory FTS spectrum of Hg II $\lambda$ 3984



# Mercury isotopic anomaly in the star HR 7775

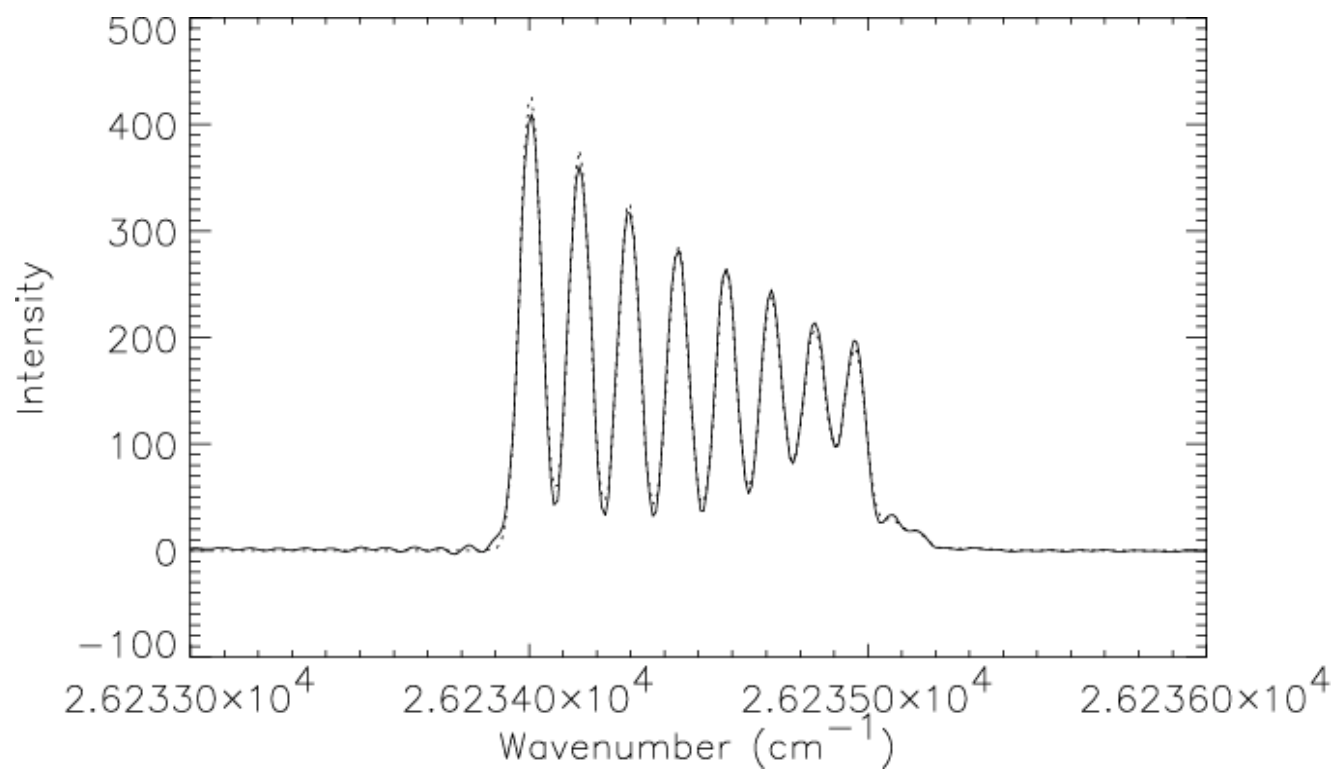


# Hyperfine structure – the splitting of energy levels

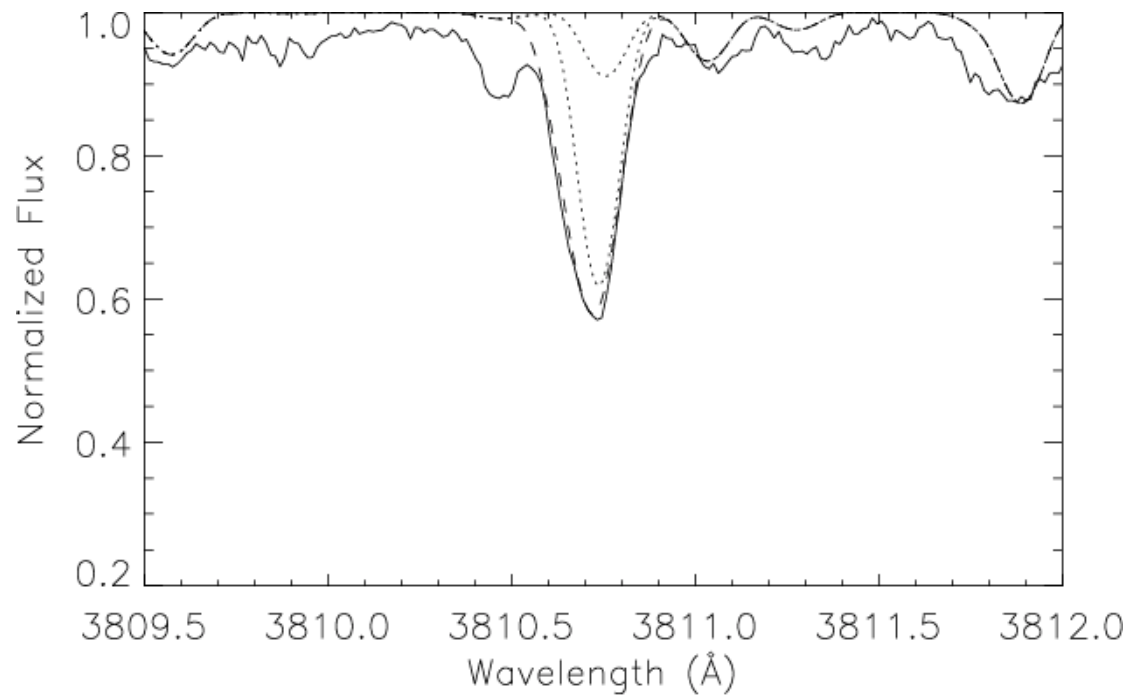


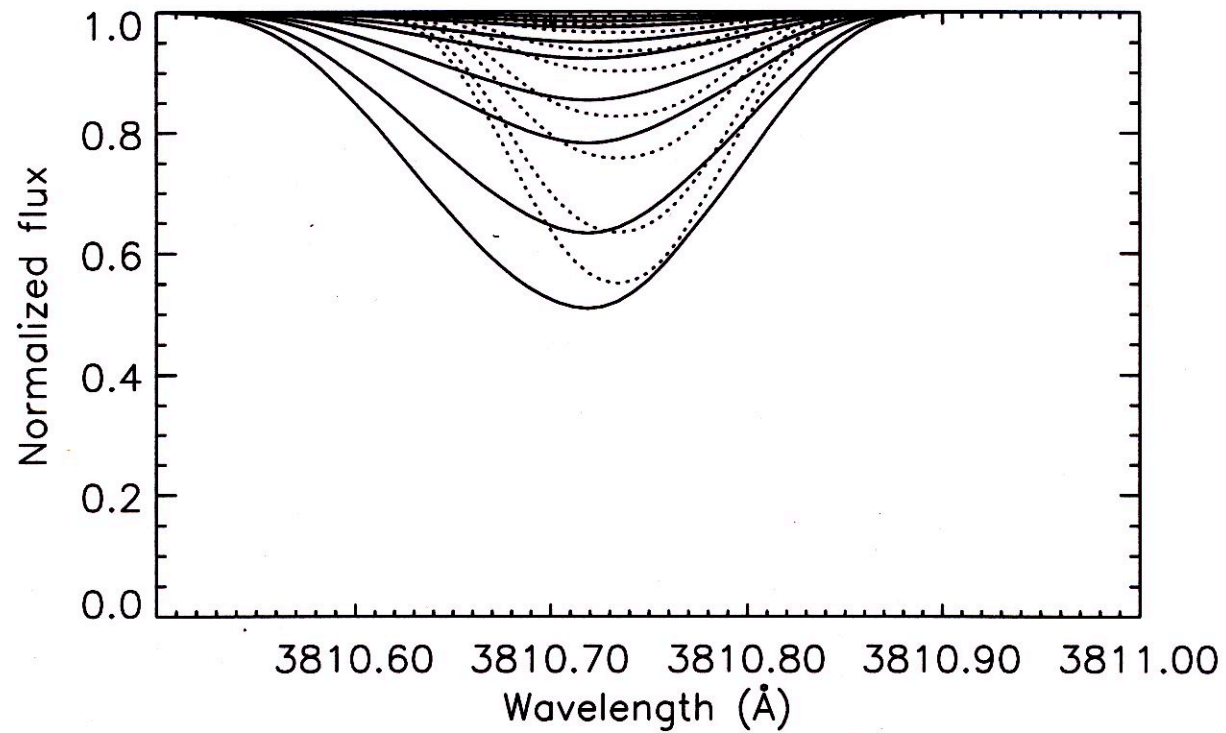
# Hyperfine structure in Ho II $\lambda 3810$

single stable isotope



## Ho II $\lambda 3810$ in the halo star CS22892-052

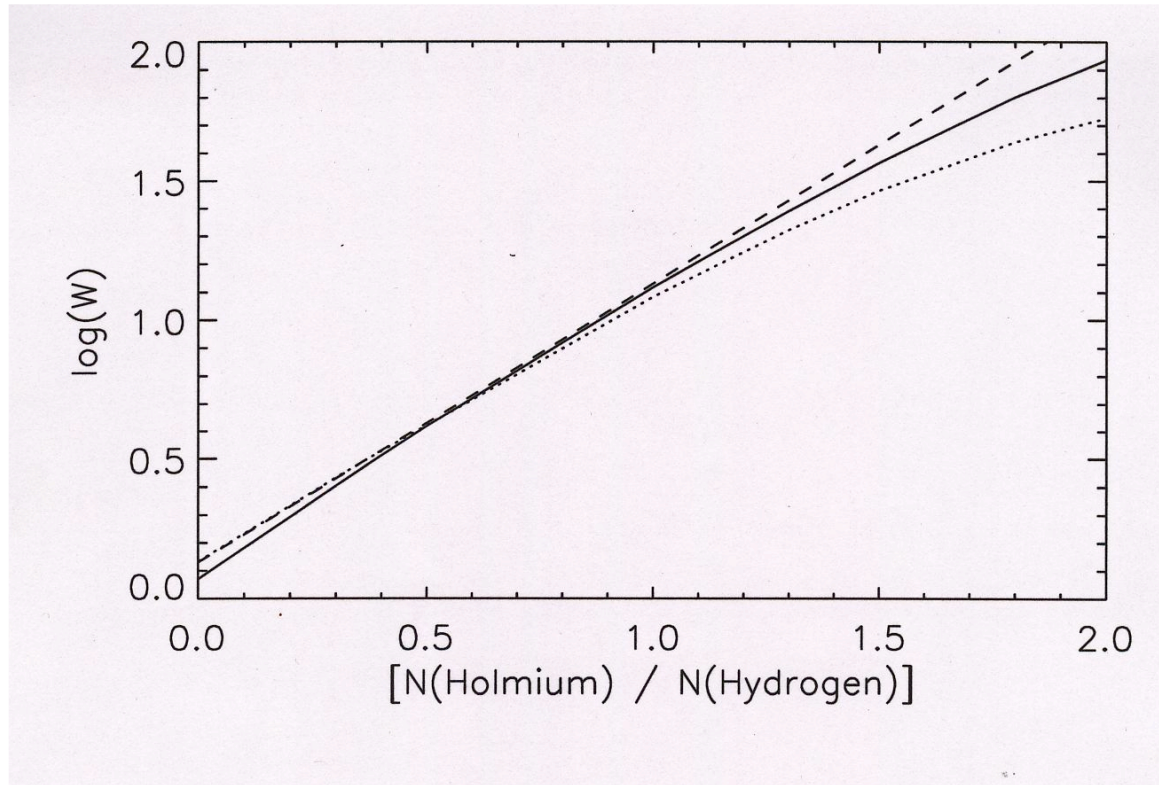




Dashed line - no hfs

Solid line - with hfs

To HFS or not to HFS - is no longer a question.



Dotted line - no hfs

Solid line - with hfs

Dashed line - unit slope, displaced +0.13 in  $\log(W)$

## Isotopes:

- \* The transition probability (and therefore) oscillator strength for a transition is the same for all isotopes of the atom/ion.
- \* In practice, we scale the  $gf$  value by the relative isotope abundances, but this would not be necessary if our synthetic spectrum codes included the abundances of individual isotopes.
- \* Therefore, if you want to change the isotope ratio, you will probably need to change the  $gf$  values accordingly.

## Combining hfs and IS effects:

$$f_{\text{line}} = f_{\text{total}} \times (A_{\text{el/isotope}} / A_{\text{el}}) \times \text{bf}_{\text{hfs}}$$



# Ex.: Decomposing the $gf$ value of $6s^2 \ ^1S_0 - 6s6p \ ^3P_1$ Tl II $\lambda 1908$

Two odd-numbered stable isotopes:  $A = 203$  (29.5%),  
 $= 205$  (69.5%)

Transition  $gf$  value =  $0.045 \pm 0.01$ , from theory

Therefore, for each isotope  $gf = 0.045$

For each isotope, hfs component  $gf$  values can be obtained by a) measured relative intensities, b) general hfs relationship using 6-j symbol, c) sum rules

| Isotope | $F_l - F_u$ | Wavelength( $\text{\AA}$ ) | $gf$ (stat. wt. ratio) |
|---------|-------------|----------------------------|------------------------|
| 203     | 0.5 - 1.5   | 1908.5632                  | 0.030                  |
|         | 0.5 - 0.5   | 1908.6982                  | 0.015                  |
| 205     | 0.5 - 1.5   | 1908.5725                  | 0.030                  |
|         | 0.5 - 1.5   | 1908.7087                  | 0.015                  |

- For use in SYNTHE, multiply isotope  $gf$  by relative isotope abundance.

$F = J + I$ ;  $I = 1/2$  for each isotope

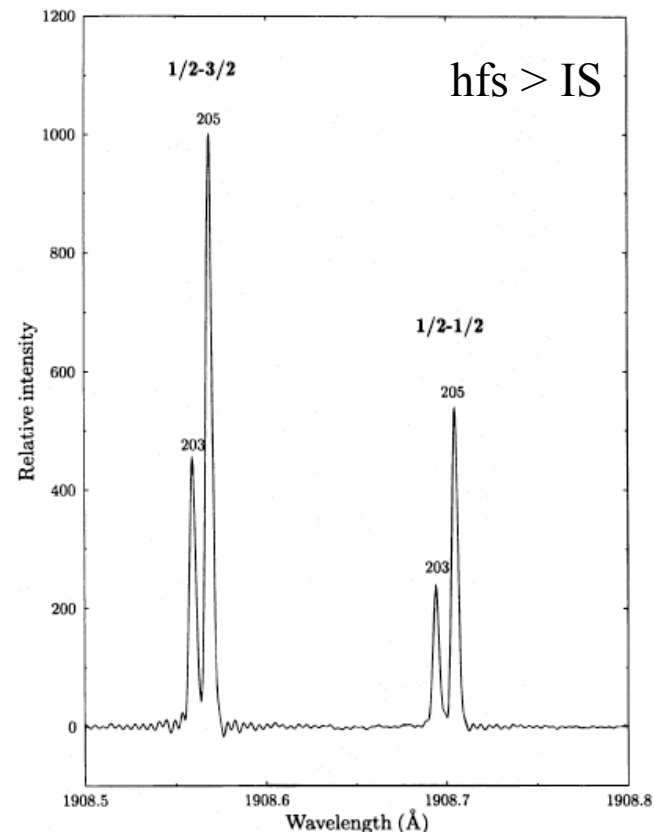


FIG. 1.—Resolved hyperfine structure and isotope shift in the inter-combination line of Tl II at 1908.6 Å, recorded with a VUV-Fourier transform spectrometer. The isotope shift of  $^{203}\text{Tl}$  and  $^{205}\text{Tl}$  is resolved for both hyperfine components,  $F = 1/2-3/2$  and  $F = 3/2-3/2$ .

(Johansson et al. 1996, ApJ 462, 943)

## VI. Uncertain(ties) comments: my point of view

- \* The uncertainty of the  $gf$  values must be considered when using a mixture of data sources. (Should one mix sources of data with different degrees of uncertainty?)
- \* Experimental data typically quote uncertainties. Try to understand what they mean. (Not all uncertainties are created equal.)
- \* Theoretical  $gf$  values may not have quoted uncertainties. (But no one would know what they mean.)
- \* Uncertainties are usually higher than quoted. (human nature)
- \* Weak lines have higher uncertainties than strong lines. (obvious)
- \* A line with a very high uncertainty may be worse for the science than not using the line. (Get a better  $f$ -value.)