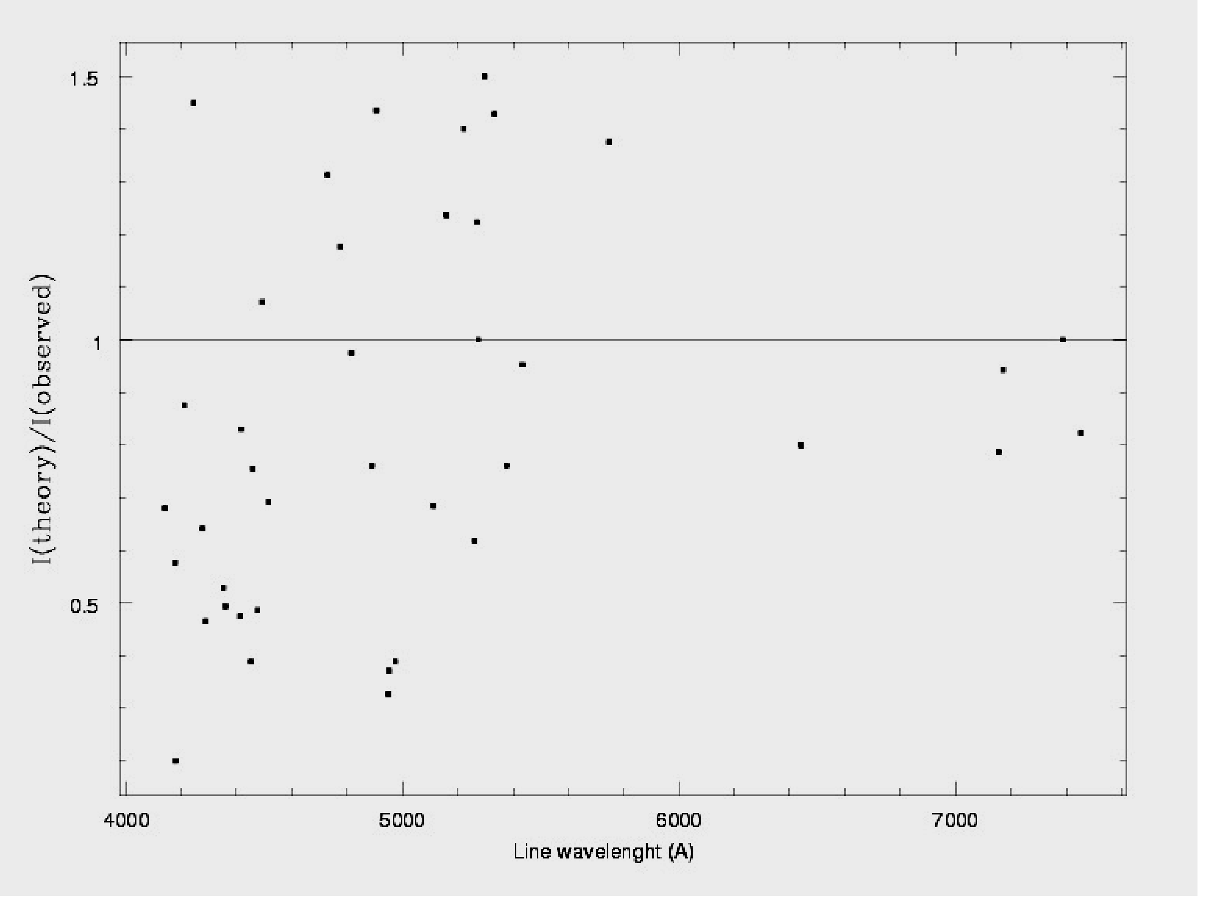
Uncertainties in Atomic Data and their Propagation through Spectral Models

Manuel Bautista and Claudio Mendoza [1]
[1]Department of Physics, Western Michigan University, Kalamazoo, MI 49008, USA
manuel.bautista@wmich.edu



Ratio of CLOUDY predicted [Fe II] line intensities to observed values in the Orion nebula (Verner et al 2000).

Modeling Fe II spectra

- A basic model for optical and IR lines needs to include the levels of the $3d^6 4s$, $3d^7$, $3d^5 4s^2$ configurations, i.e. 52 levels that yield ~1800 forbidden transitions.
- Could current theoretical methods yield accurate rates for all transitions?

How do errors in the atomic data propagate through spectral models?

Population balance equations

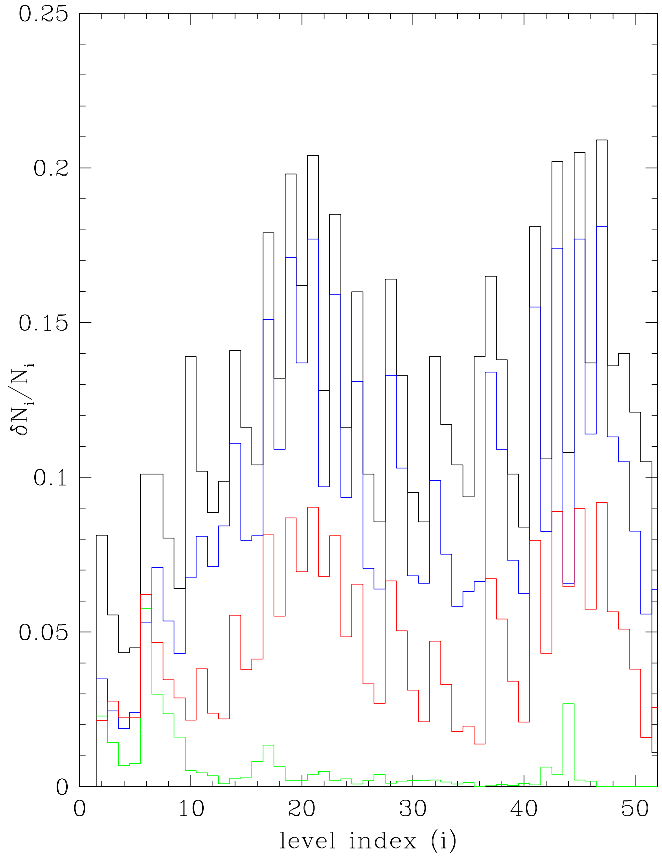
$$N_i = \frac{\sum_k N_k (n_e C_{ki} + A_{ki})}{\sum_j n_e C_{ij} + A_{ij}} = \frac{\sum_k N_k (n_e C_{ki} \tau_k + b_{ki})}{\sum_j n_e C_{ij} \tau_i + b_{ij}} \times \frac{\tau_i}{\tau_k}$$

$$\left(\frac{\delta N_i}{N_i}\right)^2 - \sum_{k\neq i} N_k^2 \frac{(n_e q_{k,i} + A_{k,i})^2}{\kappa^2}\left(\frac{\delta N_k}{N_k}\right)^2 =$$

$$\frac{1}{\kappa^2}\left[n_e^2 \sum_{k\neq i}(N_k q_{k,i} - N_i q_{i,k})^2\left(\frac{\delta \Upsilon_{k,i}}{\Upsilon_{k,i}}\right)^2 + \sum_{k>i}(N_k A_{k,i})^2\left(\frac{\delta A_{k,i}}{A_{k,i}}\right)^2 + \left(\frac{N_i^2}{\tau^2}\right)^2\left(\frac{\delta \tau_i}{\tau_i}\right)^2\right]$$

where $\kappa_i = \sum_{k\neq i} N_k(n_e q_{k,i} + A_{k,i})$.

Population uncertainties
(δτ=5%, δA=10%, δΩ=20%)



Black: total uncertainty
Blue: from collisions
Green: from lifetimes
Red: from other labels

Conclusion

- Population and ionization balance equations are linear equations, thus uncertainties from atomic parameters can be computed analytically.
- The uncertainties computations can be done very efficiently
- This allows us to analyze the sources of error in modeled spectra

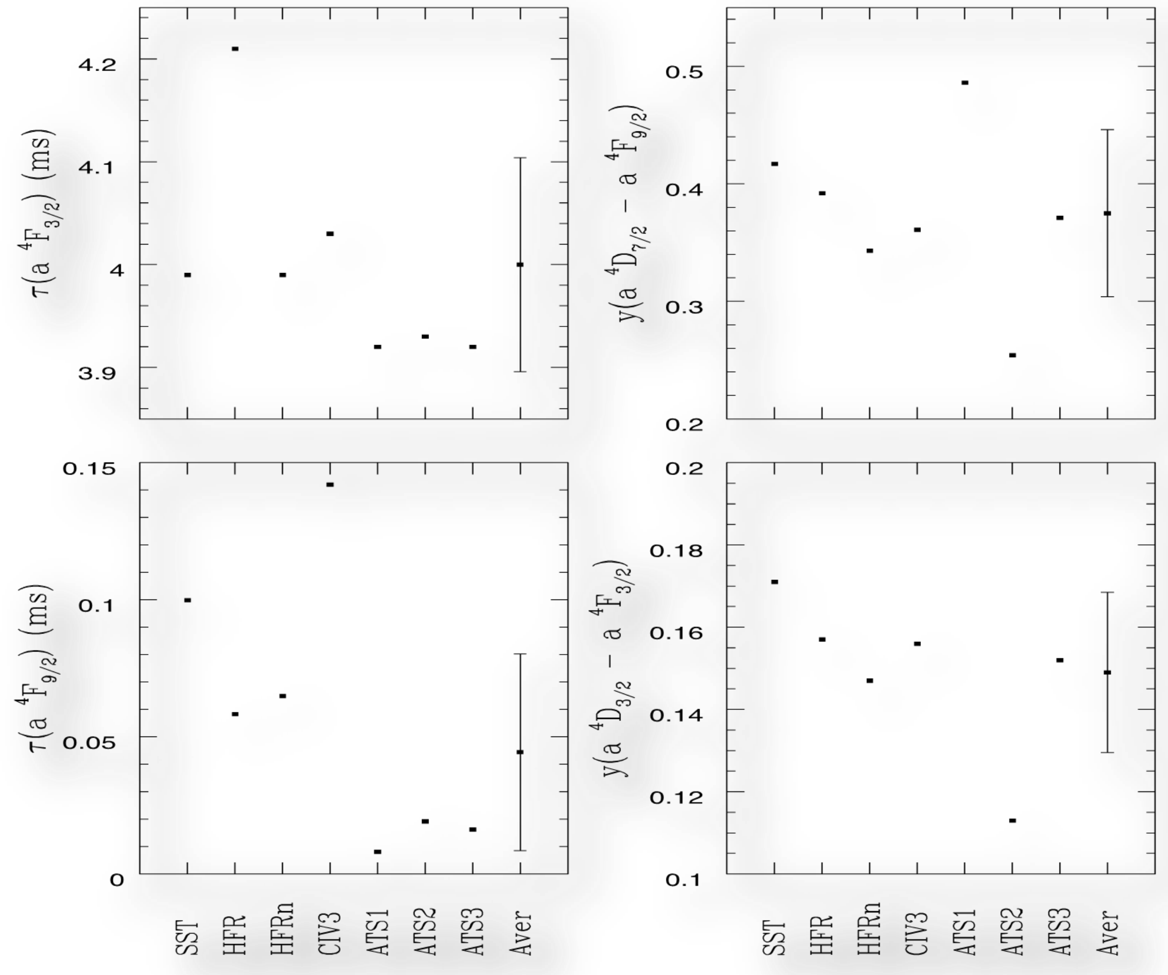
How to estimate the uncertainties in A-values?

- A-values come from theoretical calculations.
- There are numerous methods and codes.
- Our approach:
  - compare the results of different computations
  - compare with observed spectra

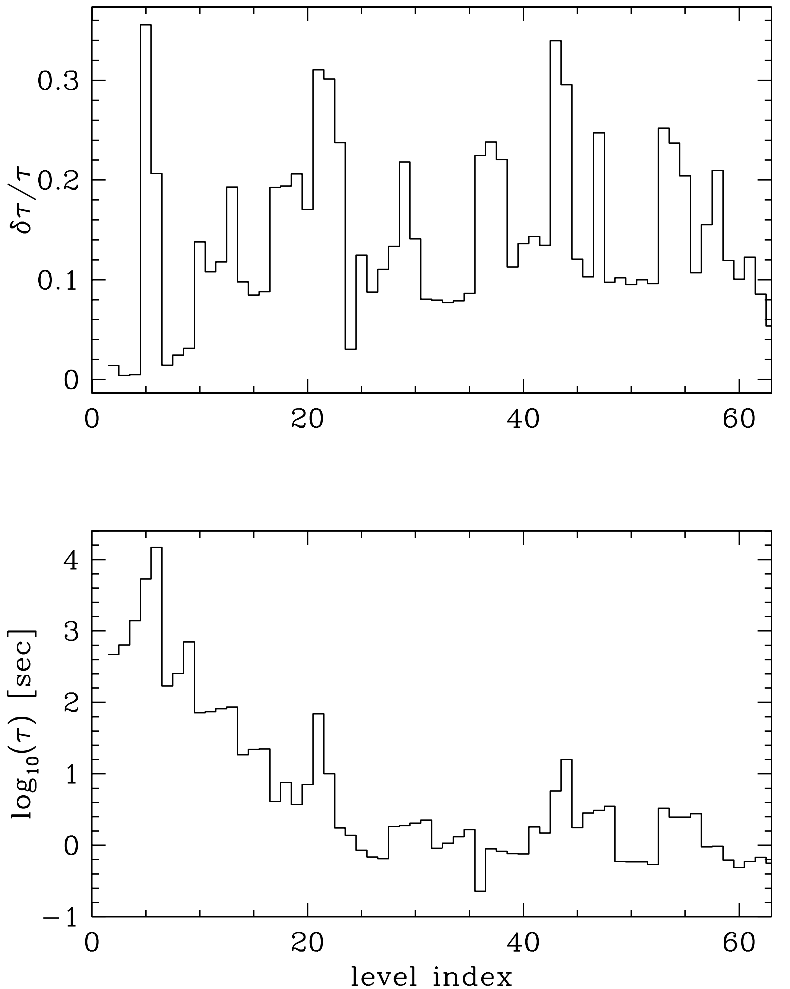
A-values

- We employ a multi-code approach: AUTOSTRUCTURE, HFR, MCDF, GRASP

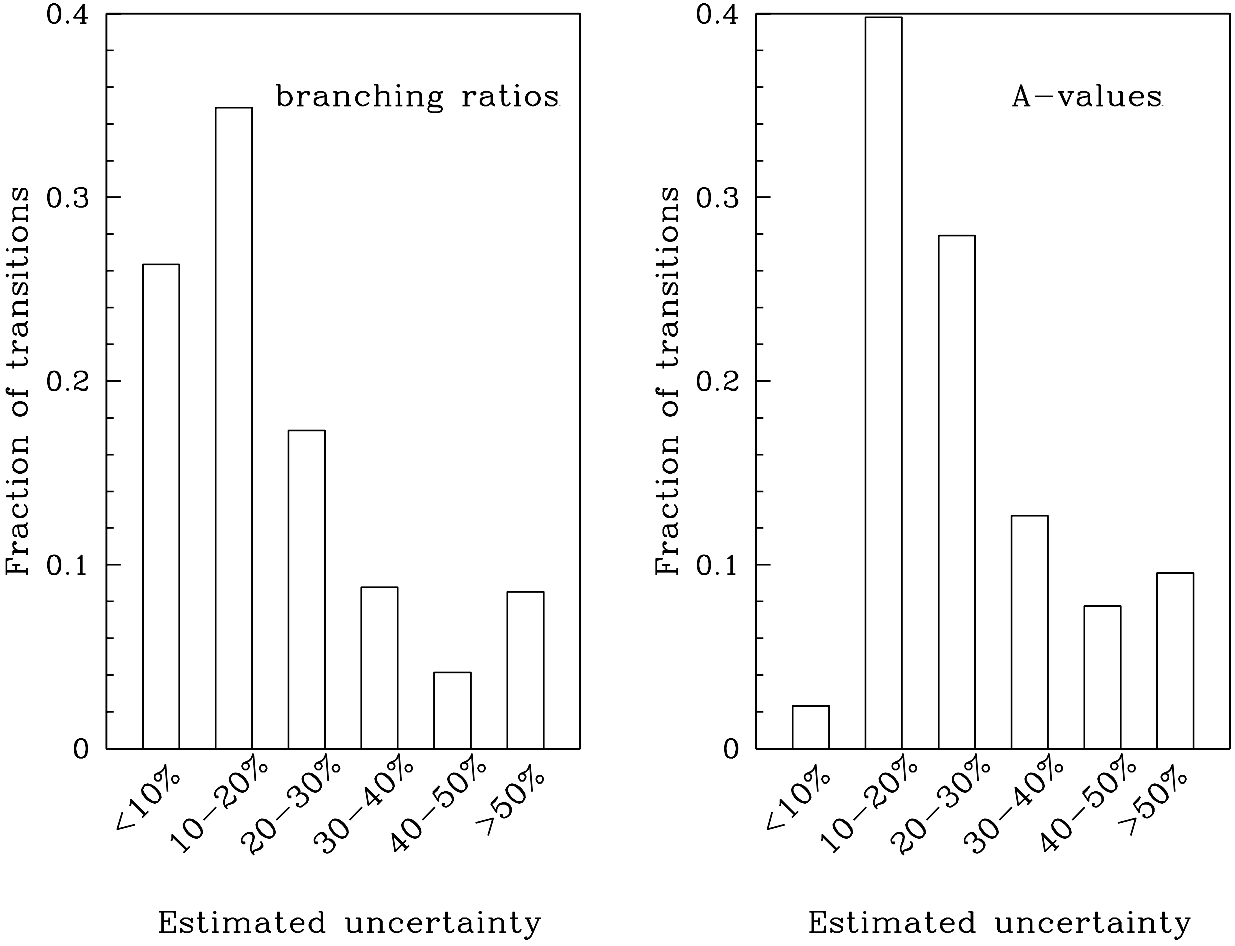
Calculated Fe II lifetimes



Lifetimes with uncertainties



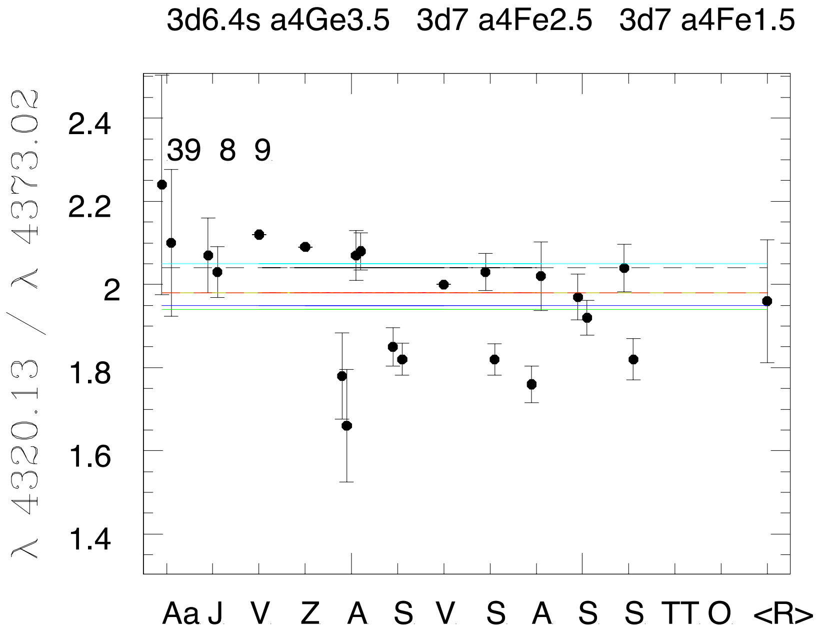
Error distribution

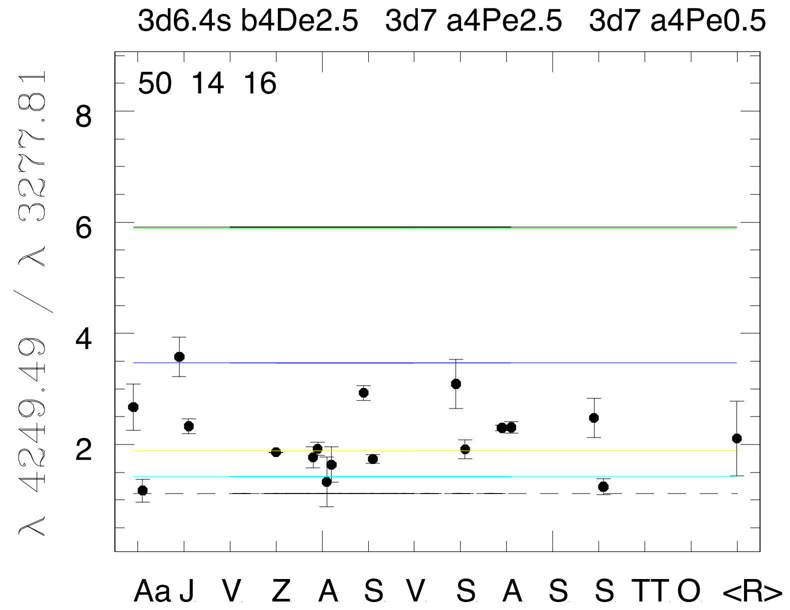


Comparisons with astronomical spectra

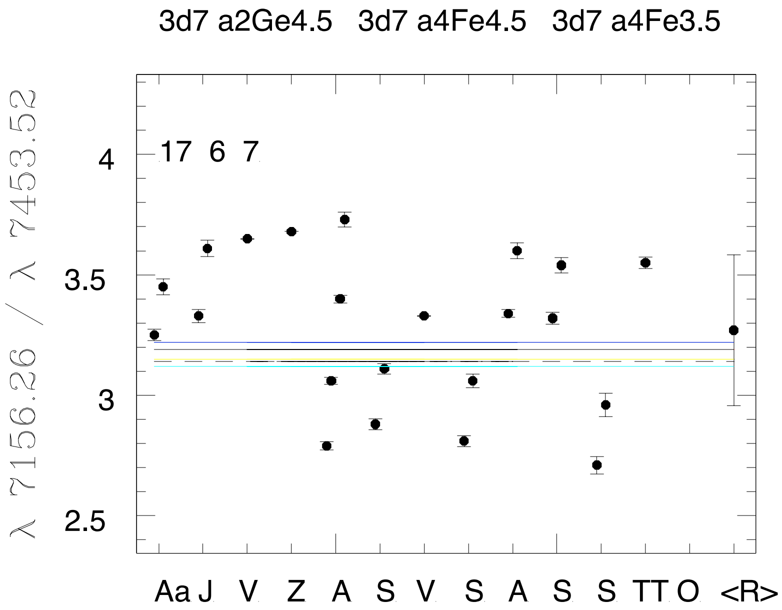
- 6 HST/STIS (3000 – 10,000 Å) spectra of the Weigelt blobs of η Carinae.
- VLT echelle (3500 – 10,000 Å) spectrum of the Orion nebula (Mesa-Delgado et al. 2009).
- X-Shooter (3000 – 25,000 Å) spectrum of the TTaury star ESO-Hα 574.

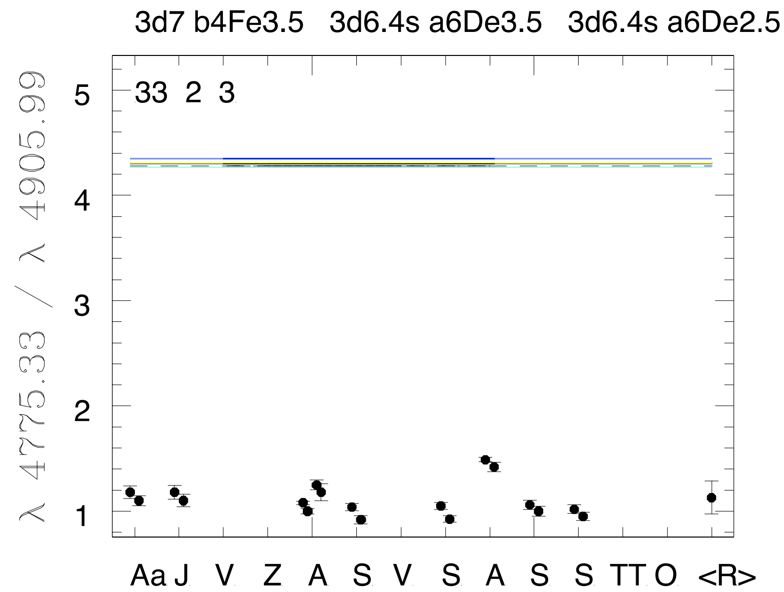
Nebular intensity ratios of lines from the same upper level and predictions from theoretical calculations of A-values.





Nebular intensity ratios of lines from the same upper level and predictions from theoretical calculations of A-values.



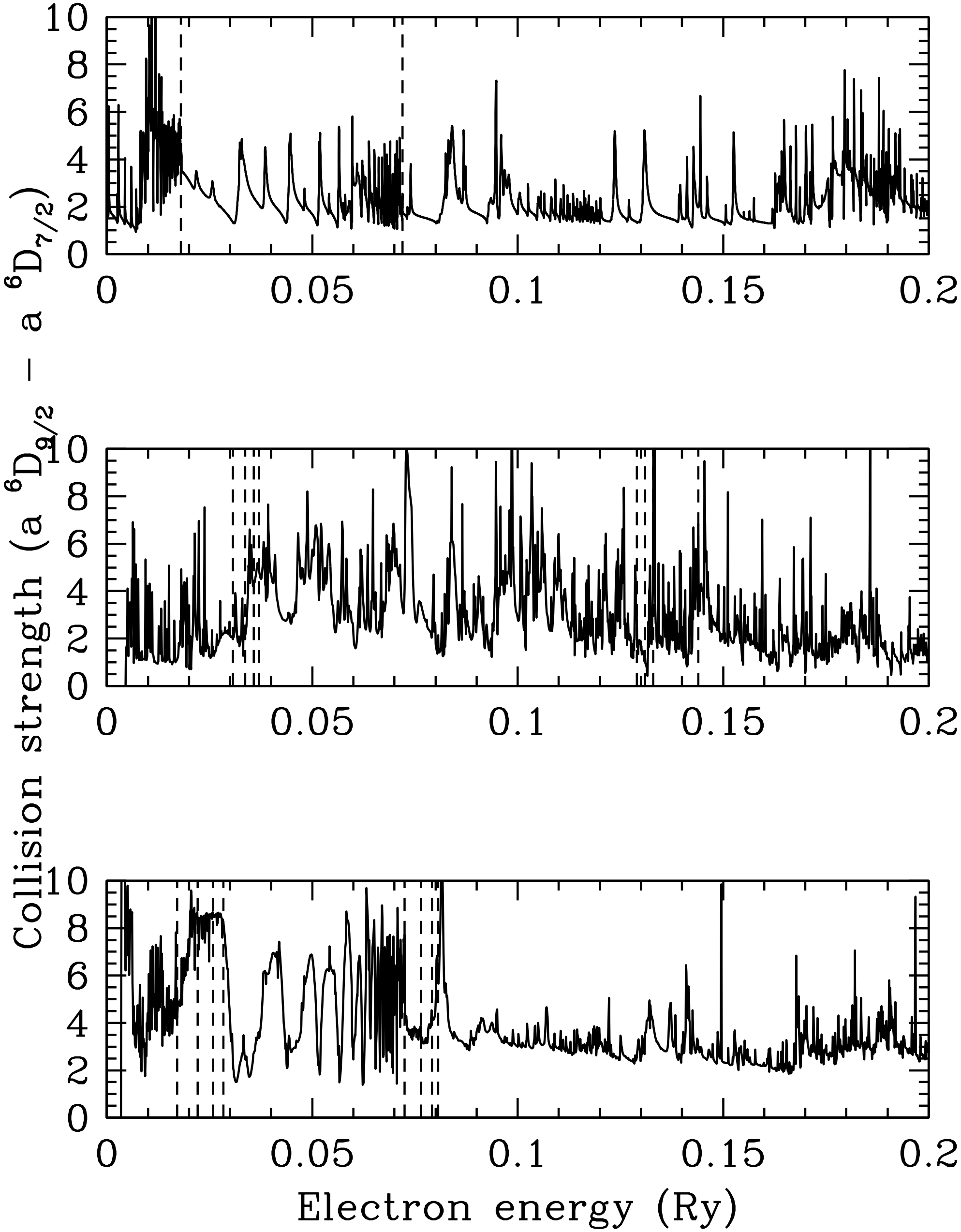


Comparison of theoretical and observed branching ratios

Calculation	χ^2
SST(QDZ96)	5.83
HFR(QDZ96)	5.09
HFR new	5.16
CIV3(DH11)	4.76
BP extend TFDAc	358
Q96+ 4d^2-corr	12.64
7-config	4.10
NewTFDAc	4.92
Recom.(δR_{th} = 0)[a]	4.34
Recommended[b]	1.38

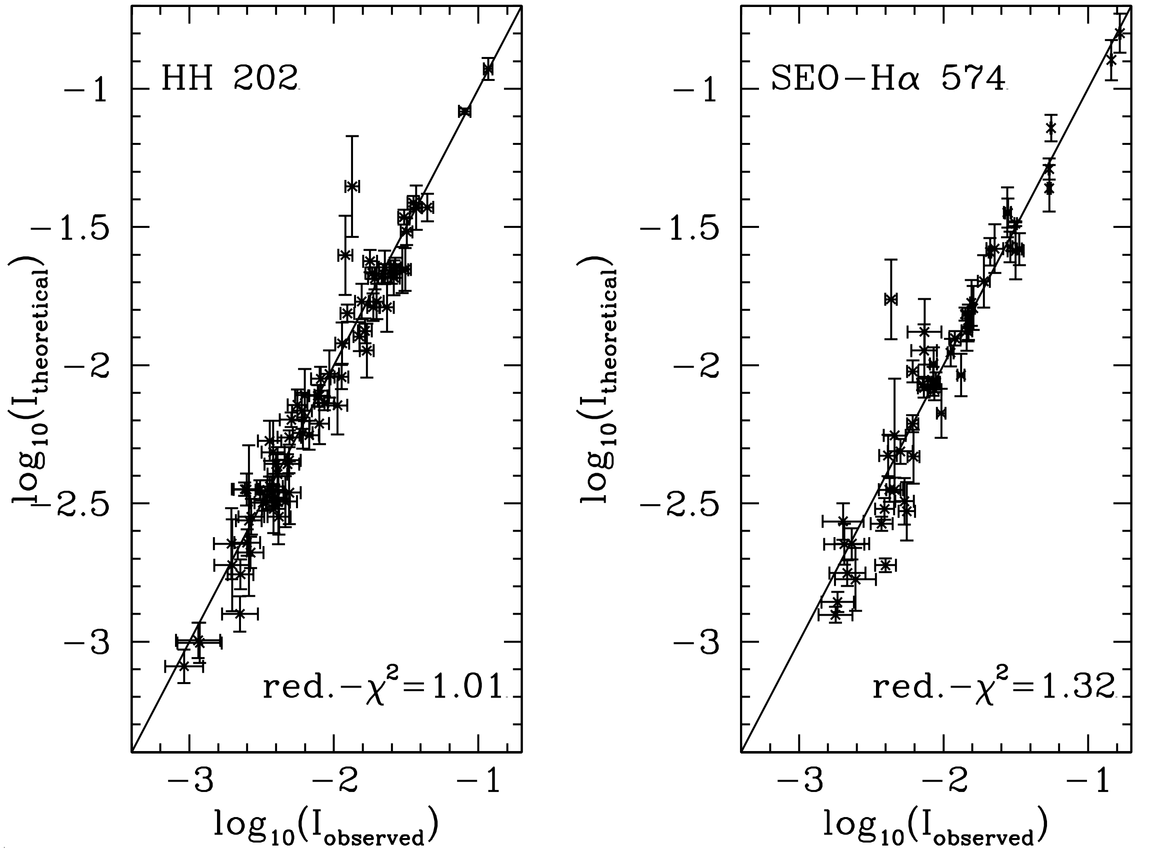
Table 8. Effective collision strengths from the ground level of [Fe II] at 10^4 K

j	Q+RM[a]	Q+RM[b]	Q+RM[c]	Q+RM[d]	7-config[e]	DARC[f]	Mean[g]	σ[h]	ZP96[i]	BP96[k]	RH07[k]
2	1.81+0	2.05+0	2.80+0	2.24+0	2.85+0	5.16+0	2.31+0	16.0	5.52+0	4.65+0	4.84+0
3	3.36−1	3.89−1	6.52−1	4.93−1	4.20−1	1.20+0	4.21−1	23.8	1.49+0	1.29+0	1.12+0
4	1.54−1	1.58−1	3.58−1	2.33−1	1.78−1	5.11−1	1.95−1	35.3	6.84−1	8.13−1	5.29−1
5	7.16−2	7.33−2	1.81−1	1.16−1	8.57−2	2.22−1	9.51−2	37.8	2.84−1	.337−1	2.47−1



Collision strength (a 6D9/2 − a 6D7/2)
10
8
6
4
2
0
0
0.05
0.1
0.15
0.2
Electron energy (Ry)

Calculated vs. Observed line intensities.



Conclusion

- Atomic data (theoretical or experimental) have limited accuracy:

  -‘Newer’ data does NOT mean ‘better’ data

  -No one atomic/molecular calculation can provide accurate results for every rate

  -The data set from the ‘most accurate’ calculation may NOT give you the best spectral model

What to do?

- Consider ALL data sets available (the good, the bad, and the ugly)
- Estimate uncertainties for every rate individually
- Build a basis data set
- Look for critically important rates
- Focus on those specifically

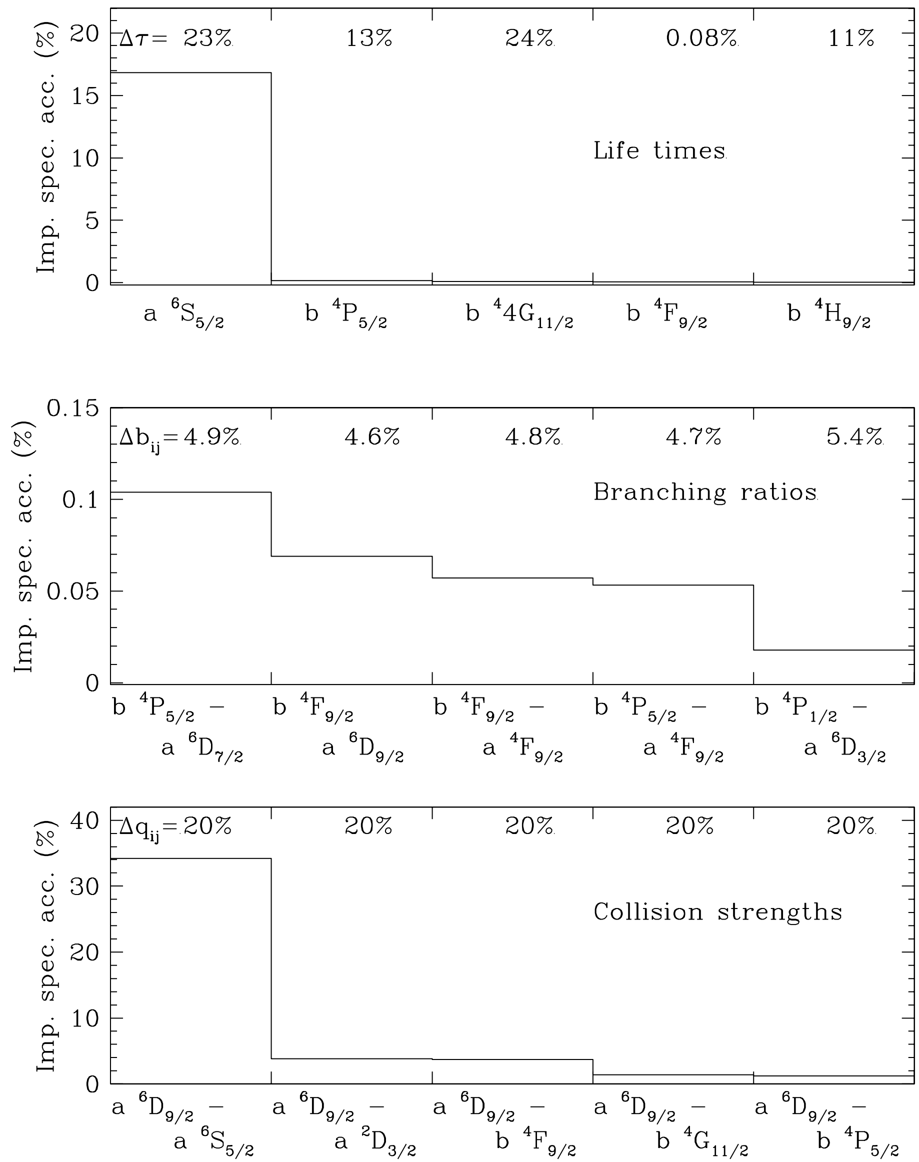
Spectrum average uncertainty

$$\Delta j_{aver} = \frac{\sum_i j_i^2 \Delta j_i}{\sum_i j_i^2}$$

- For FeII in the range 3000Å to 4000Å,

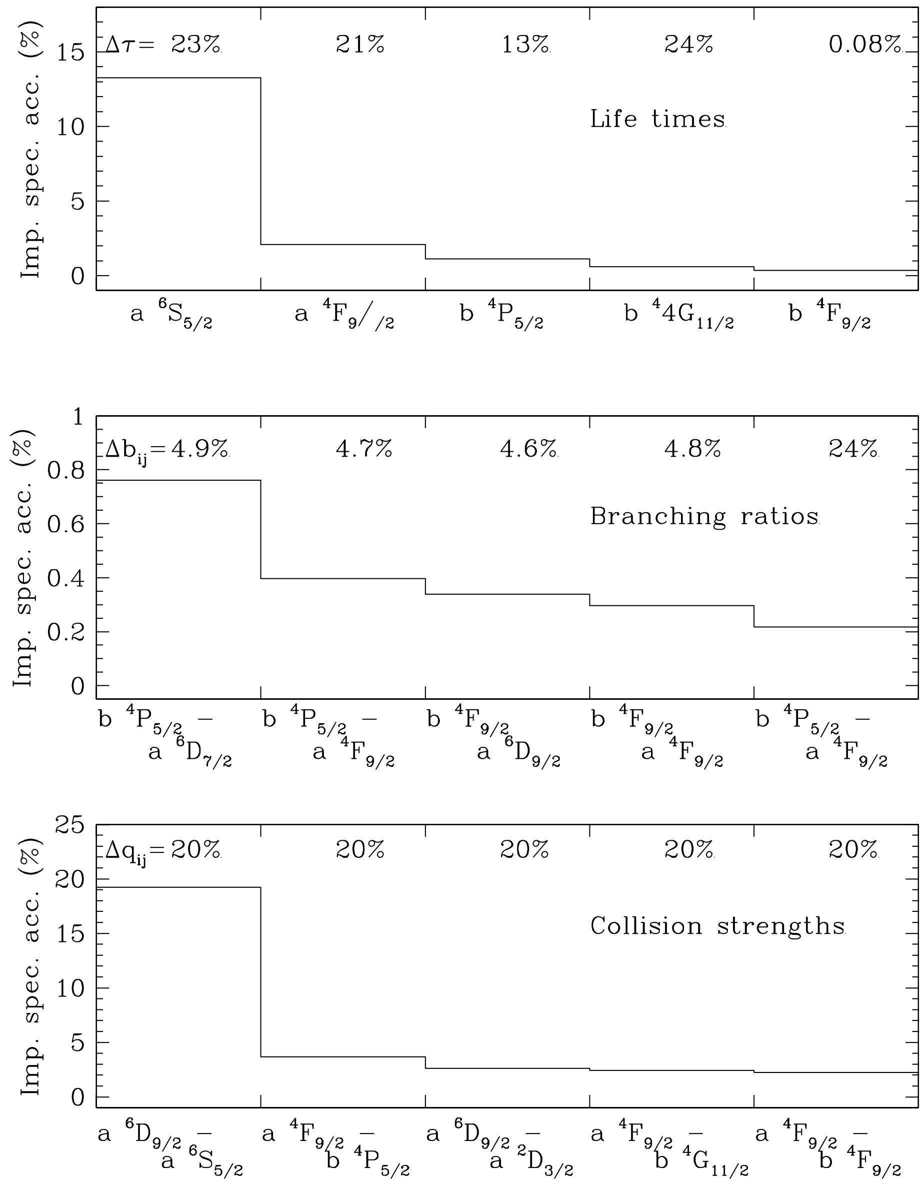
$$\Delta j_{aver} \approx 21\%$$

$n_e=10^1\ cm^{-3}$



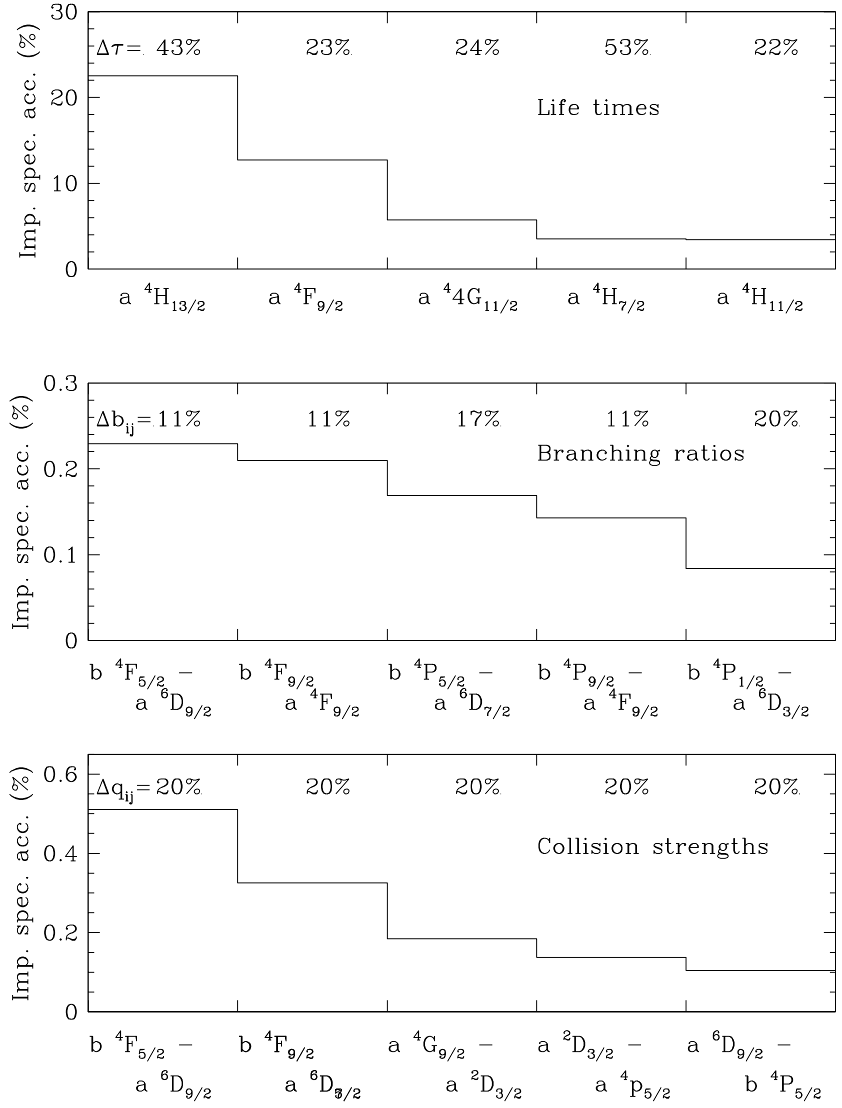
Imp. spec. acc. (%)
Δτ= 23%
13%
24%
0.08%
11%
Life times
a $^6S_{5/2}$
b $^4P_{5/2}$
b $^44G_{11/2}$
b $^4F_{9/2}$
b $^4H_{9/2}$
Δb$_{ij}$=4.9%
4.6%
4.8%
4.7%
5.4%
Branching ratios
b $^4P_{5/2}$ – a $^6D_{7/2}$
b $^4F_{9/2}$ a $^6D_{9/2}$
b $^4F_{9/2}$ – a $^4F_{9/2}$
b $^4P_{5/2}$ – a $^4F_{9/2}$
b $^4P_{1/2}$ – a $^6D_{3/2}$
Δq$_{ij}$=20%
20%
20%
20%
20%
Collision strengths
a $^6D_{9/2}$ – a $^6S_{5/2}$
a $^6D_{9/2}$ – a $^2D_{3/2}$
a $^6D_{9/2}$ – b $^4F_{9/2}$
a $^6D_{9/2}$ – b $^4G_{11/2}$
a $^6D_{9/2}$ – b $^4P_{5/2}$

$n_e=10^3$ cm^{-3}



Imp. spec. acc. (%)
Δτ= 23%
21%
13%
24%
0.08%
Life times
a 6S5/2
a 4F9/ /2
b 4P5/2
b 44G11/2
b 4F9/2
Imp. spec. acc. (%)
Δbij=4.9%
4.7%
4.6%
4.8%
24%
Branching ratios
b 4P5/2 – a 6D7/2
b 4P5/2 – a 4F9/2
b 4F9/2 a 6D9/2
b 4F9/2 a 4F9/2
b 4P5/2 – a 4F9/2
Imp. spec. acc. (%)
Δqij=20%
20%
20%
20%
20%
Collision strengths
a 6D9/2 – a 6S5/2
a 4F9/2 – b 4P5/2
a 6D9/2 – a 2D3/2
a 4F9/2 – b 4G11/2
a 4F9/2 – b 4F9/2

$n_e = 10^7$ cm^{-3}



Imp. spec. acc. (%)
Δτ= 43%
23%
24%
53%
22%
Life times
a ⁴H13/2
a ⁴F9/2
a ⁴4G11/2
a ⁴H7/2
a ⁴H11/2
Δbij= 11%
11%
17%
11%
20%
Branching ratios
b ⁴F5/2 – a ⁶D9/2
b ⁴F9/2 a ⁴F9/2
b ⁴P5/2 – a ⁶D7/2
b ⁴P9/2 – a ⁴F9/2
b ⁴P1/2 – a ⁶D3/2
Δqij= 20%
20%
20%
20%
20%
Collision strengths
b ⁴F5/2 – a ⁶D9/2
b ⁴F9/2 a ⁶D3/2
a ⁴G9/2 – a ²D3/2
a ²D3/2 – a ⁴p5/2
a ⁶D9/2 – b ⁴P5/2

- We are building an atomic data CURATION tool (AtomPy) that will provide uncertainties for all rates and a spectra analysis tool with propagation of uncertainties.