Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities

Alexander Kramida

National Institute of Standards and Technology, Gaithersburg, MD, USA

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Outline

- Data sources
- Evaluation of wavelengths and energy levels
- Evaluation of transition probabilities

Data sources

- Bibliographic Databases:
  - NIST Atomic Energy Levels Bibliographic Database,

    http://physics.nist.gov/Elevbib

  - NIST Atomic Transition Probability Bibliographic Database,

    http://physics.nist.gov/Fvalbib

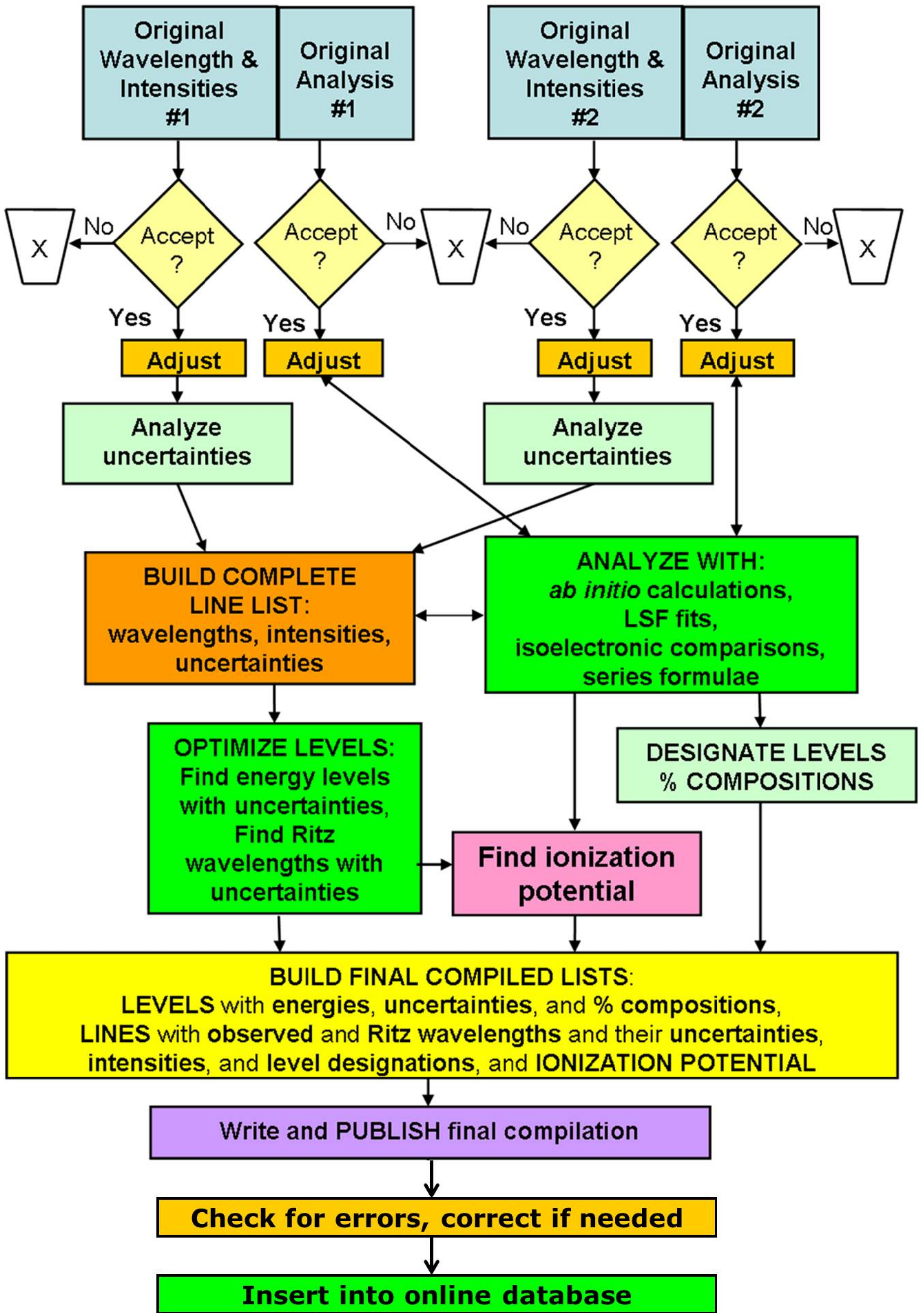
  - BIBL: Bibliography Database on Atomic Spectra,

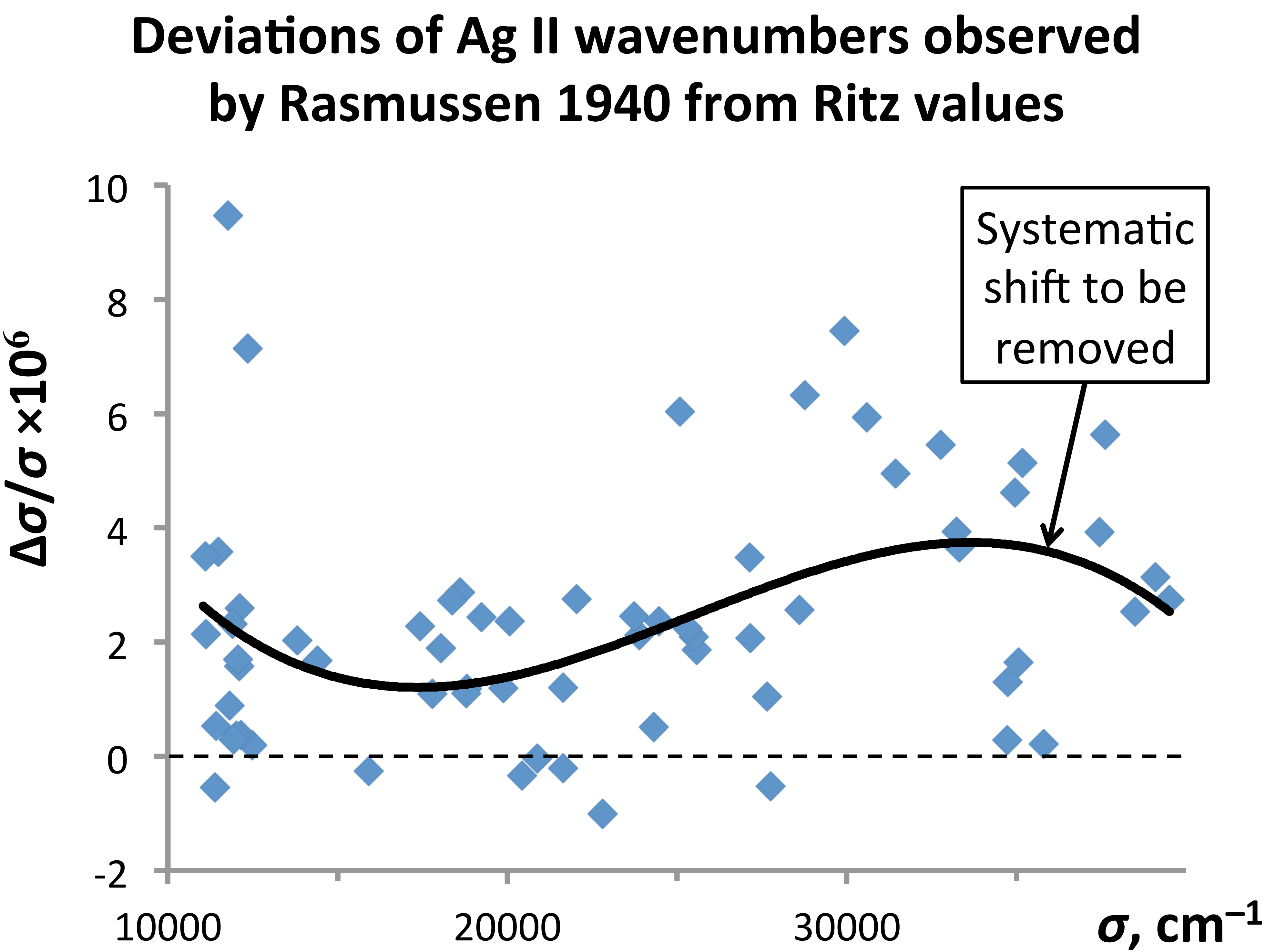
    http://das101.isan.troitsk.ru/bibl.htm

Evaluation of wavelengths and energy levels

- General workflow
- Evaluation of wavelengths
- Evaluation of intensities
- Evaluation of consistency of analysis
- Level optimization
- Deriving ionization energy
- Theoretical interpretation of levels
- Isoelectronic comparisons

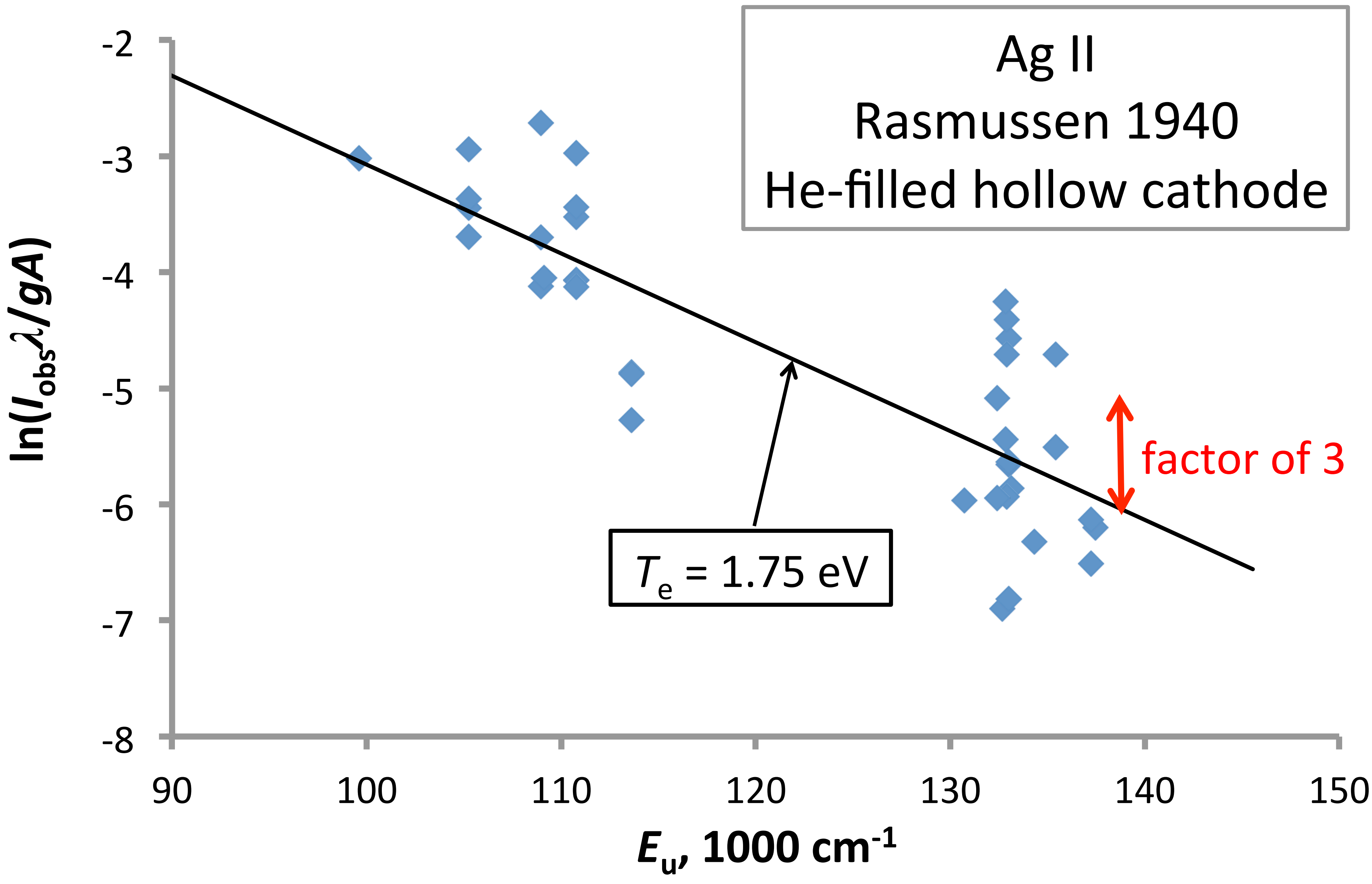
Workflow of critical evaluation of data on wavelengths and energy levels



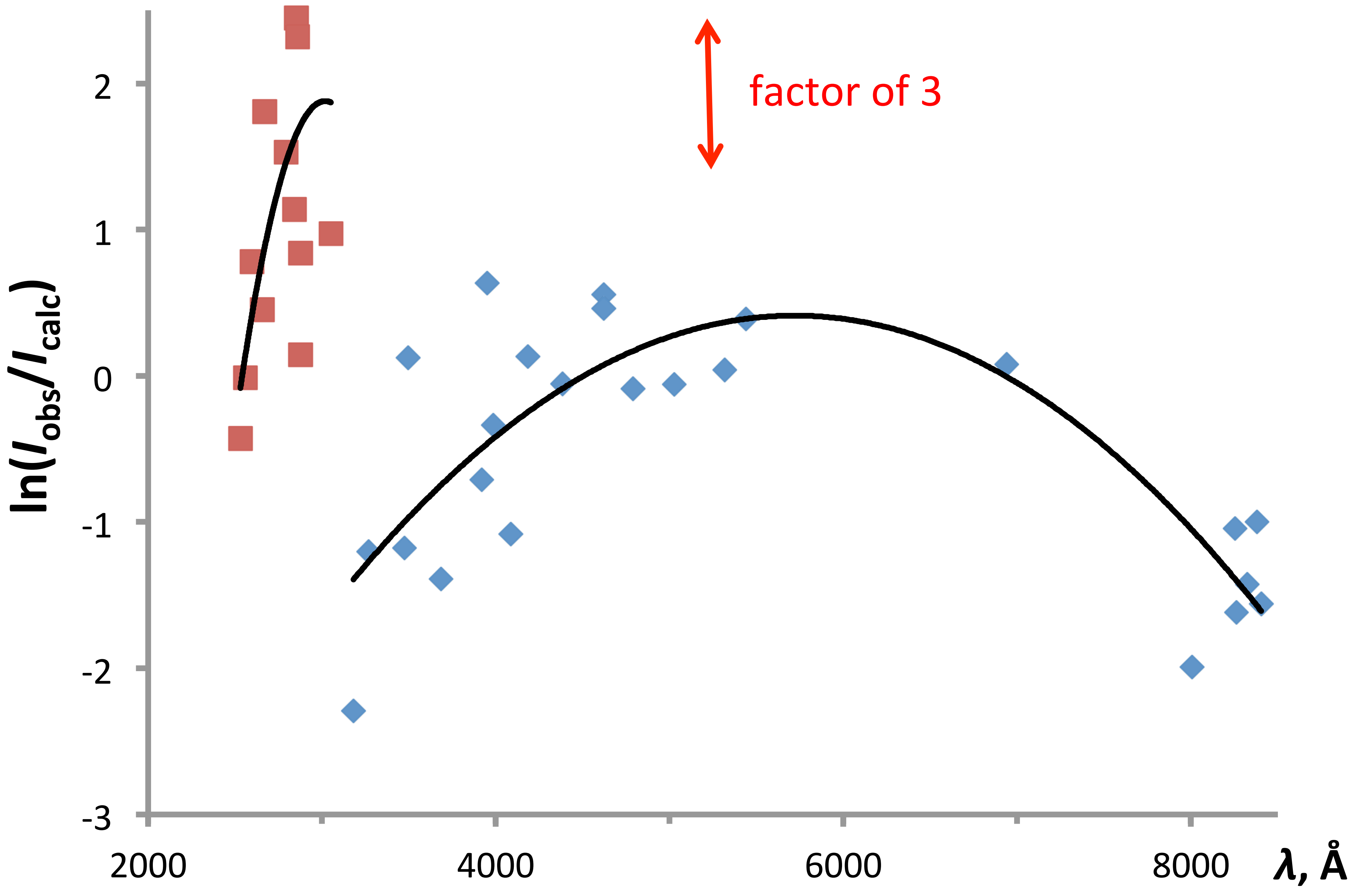


Deviations of Ag II wavenumbers observed
by Rasmussen 1940 from Ritz values
Systematic shift to be removed
Δσ/σ ×10⁶
σ, cm⁻¹
10
8
6
4
2
0
-2
10000
20000
30000

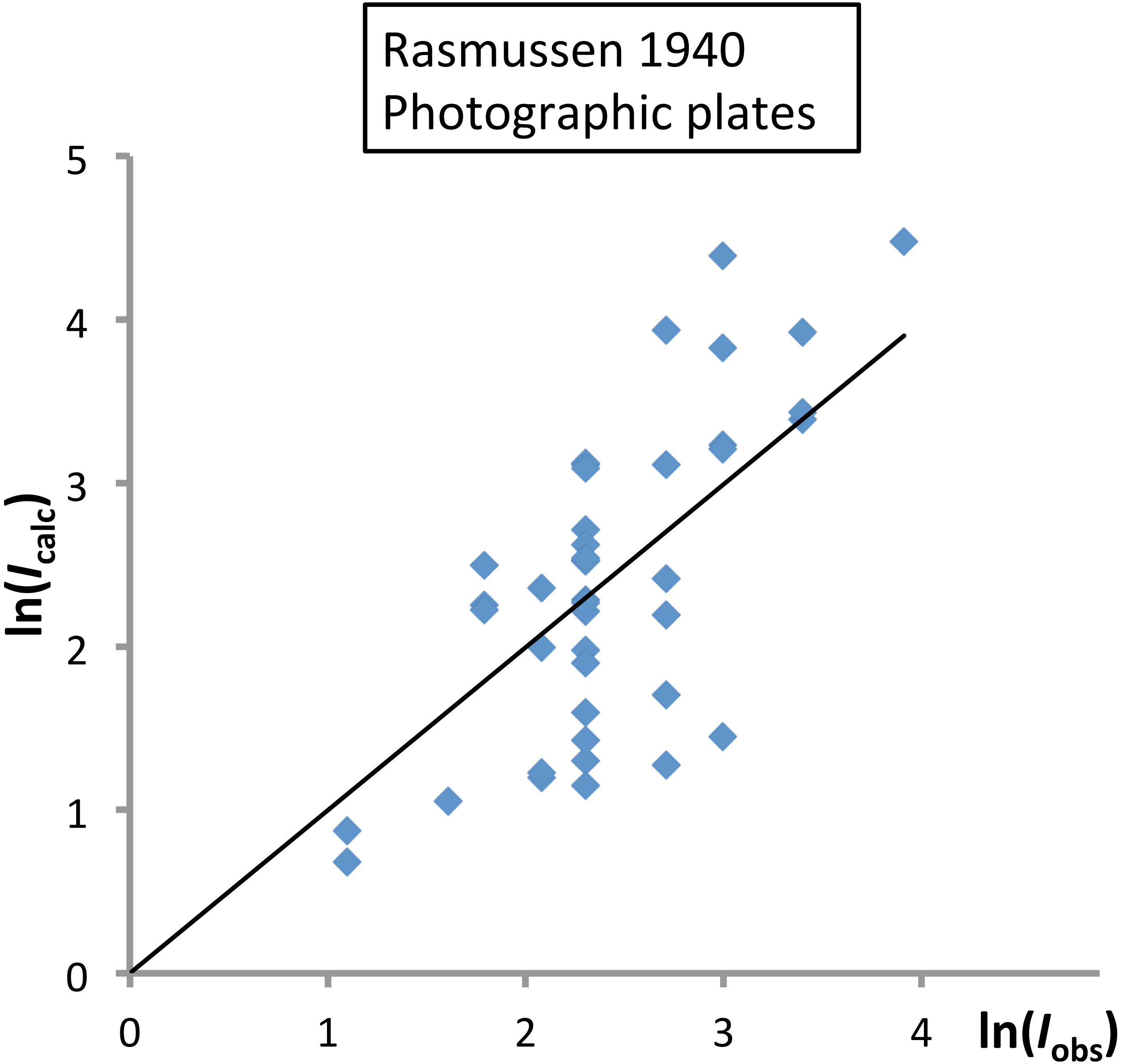
Evaluation of line intensities: Deriving excitation temperature from a Boltzmann plot



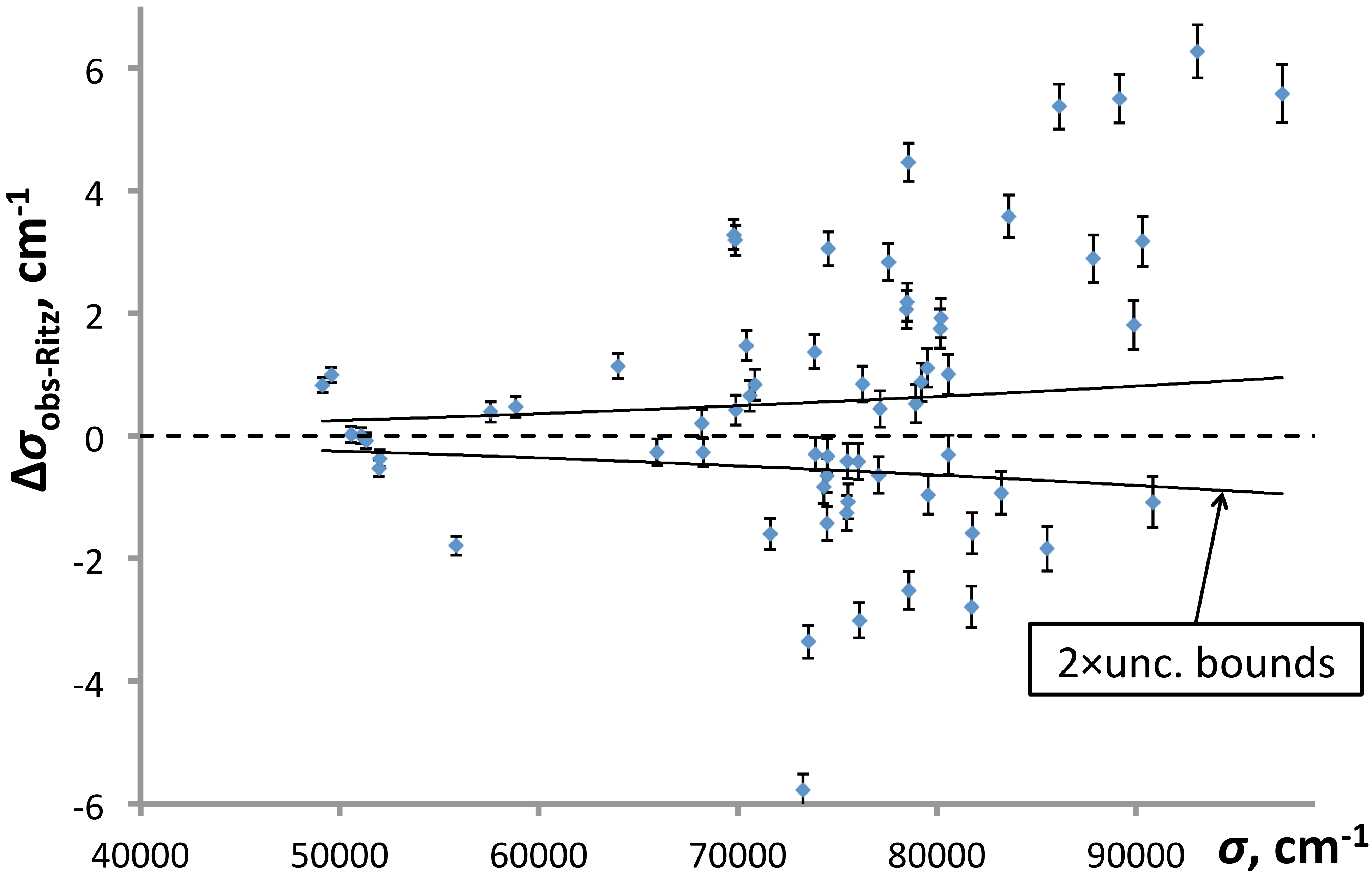
Spectral response calibration for Rasmussen 1940

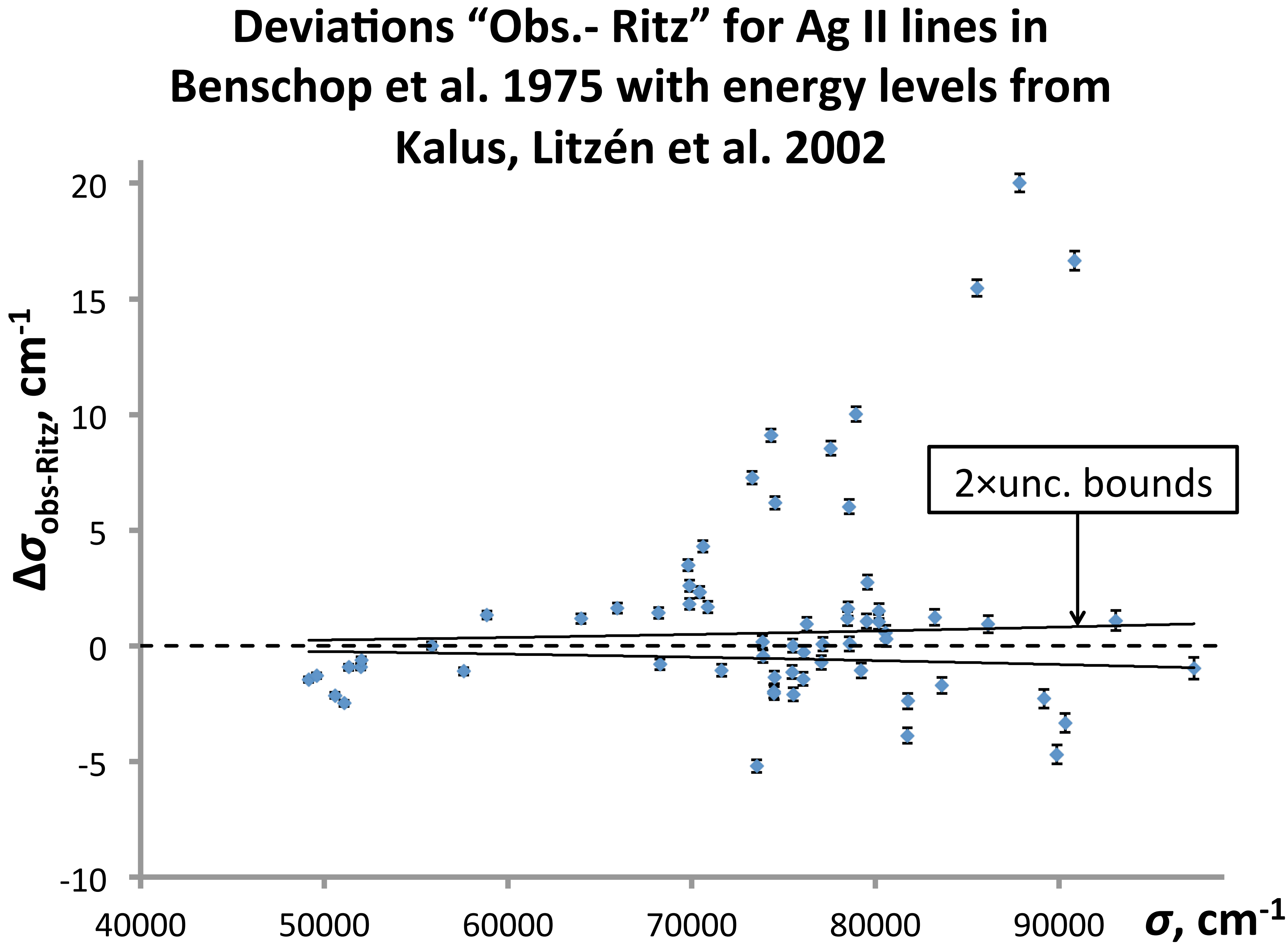


Verification of linearity of intensity scale



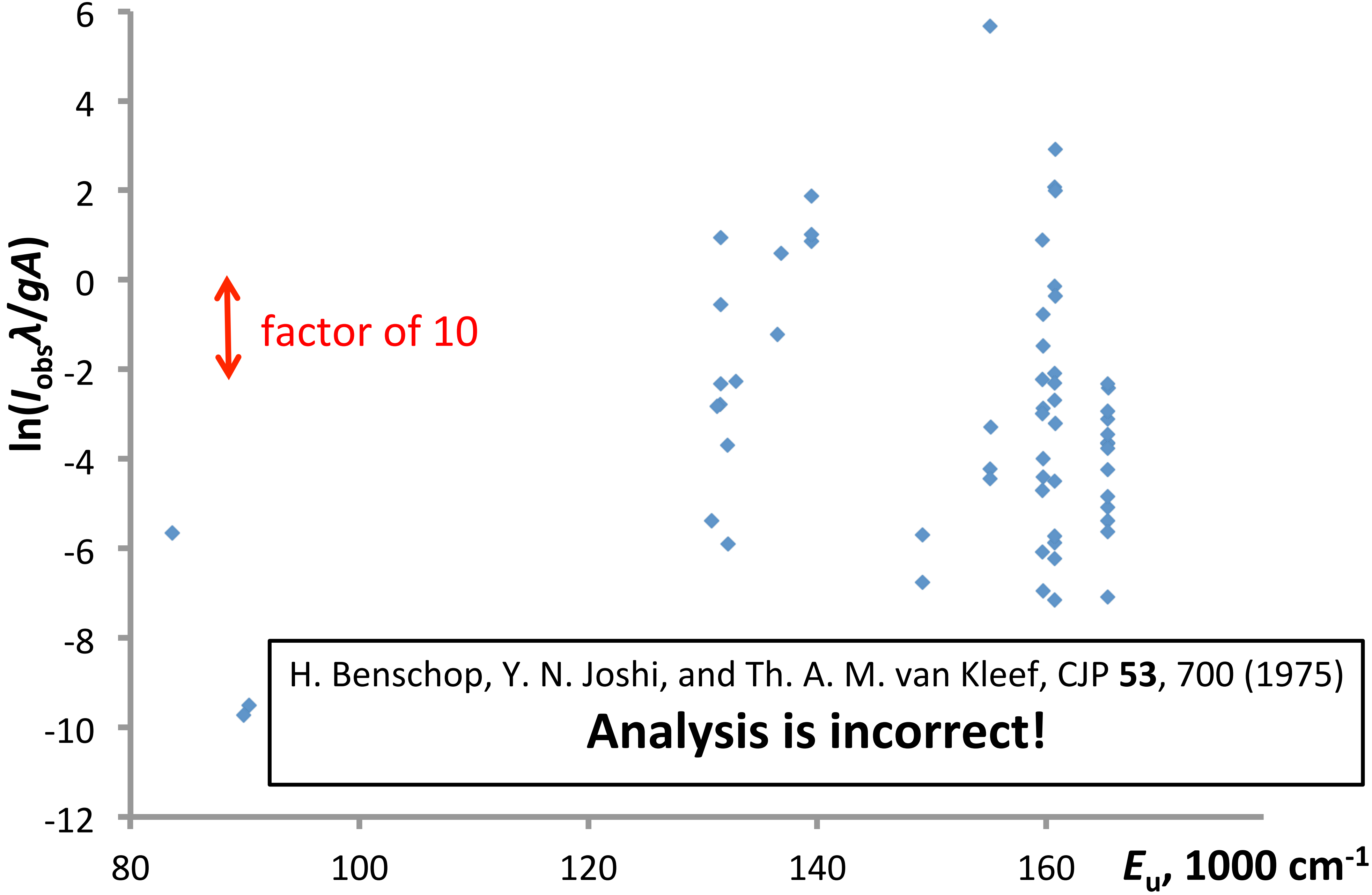
Deviations "Obs.-Ritz" for Ag II lines in Benschop et al. 1975 with their energy levels





Deviations "Obs.- Ritz" for Ag II lines in
Benschop et al. 1975 with energy levels from
Kalus, Litzén et al. 2002
$\Delta\sigma_{obs\text{-}Ritz}$, cm^{-1}
20
15
10
5
0
-5
-10
40000
50000
60000
70000
80000
90000
σ, cm^{-1}
2×unc. bounds

Boltzmann plot of Ag II line intensities observed by Benschop et al. 1975



Least squares level optimization:

Code LOPT, A. Kramida, CPC **182**, 419 (2011)

Deriving ionization energy:

From Rydberg series quantum defects –

Code RITZPL by C. J. Sansonetti

From polarization formula –

Code POLAR by C. J. Sansonetti

Semiempirical methods (various)

Theoretical interpretation of levels:

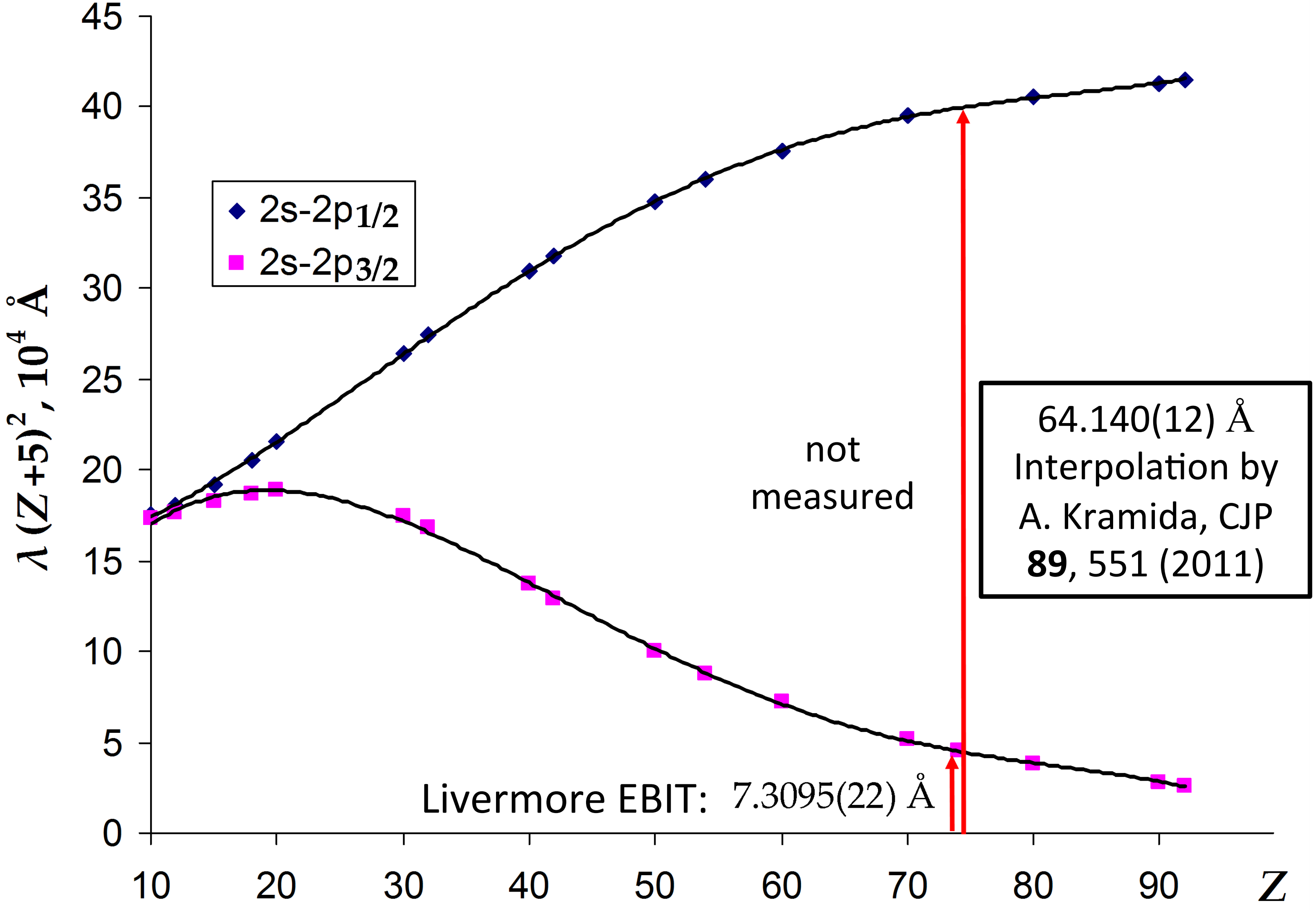
Cowan codes,

R. D. Cowan, *The Theory of Atomic Structure and Spectra*, University of California Press, Berkeley, CA (1981).

Kramida's version for Windows: http://das101.isan.troitsk.ru/COWAN

Isoelectronic comparisons

Example: Resonance lines of Li-like ions



Evaluation of transition probabilities

- Checking critical factors
- Matching calculated TP with experimental energy levels
- Matching different calculations with each other
- Selecting best TP values
- Checking for regularities

Critical factors in TP evaluation

Theory:

- Configuration interaction
- Near coincidences of energy levels
- Cancellation effects
- Relativistic corrections
- Convergence of results and of length and velocity forms

Experiment (emission spectroscopy):

- Validity of the plasma model
- Self-absorption effects
- Spectral calibration of intensities

Experiment (lifetime measurements):

- Selective excitation, cascades
- Collisional effects and radiation trapping
- Absence of line blending
- Polarization effects and quantum beats

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The Critical Assessment of Atomic Oscillator Strengths

W. L. Wiese

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

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Abstract

During the course of critical compilations of atomic oscillator strengths at the National Institute of Standards and Technology over the last 30 years, we have developed and refined a general scheme to assess the accuracy of the pertinent experimental and theoretical data. To arrive at the accuracy ratings, we have utilized general assessments of the various approaches, the attention the authors give to the critical factors of their method, the authors' uncertainty estimates, extensive data comparisons, and fits into systematic trends. Some examples will be shown which indicate that accuracy estimates in the literature are often too optimistic.

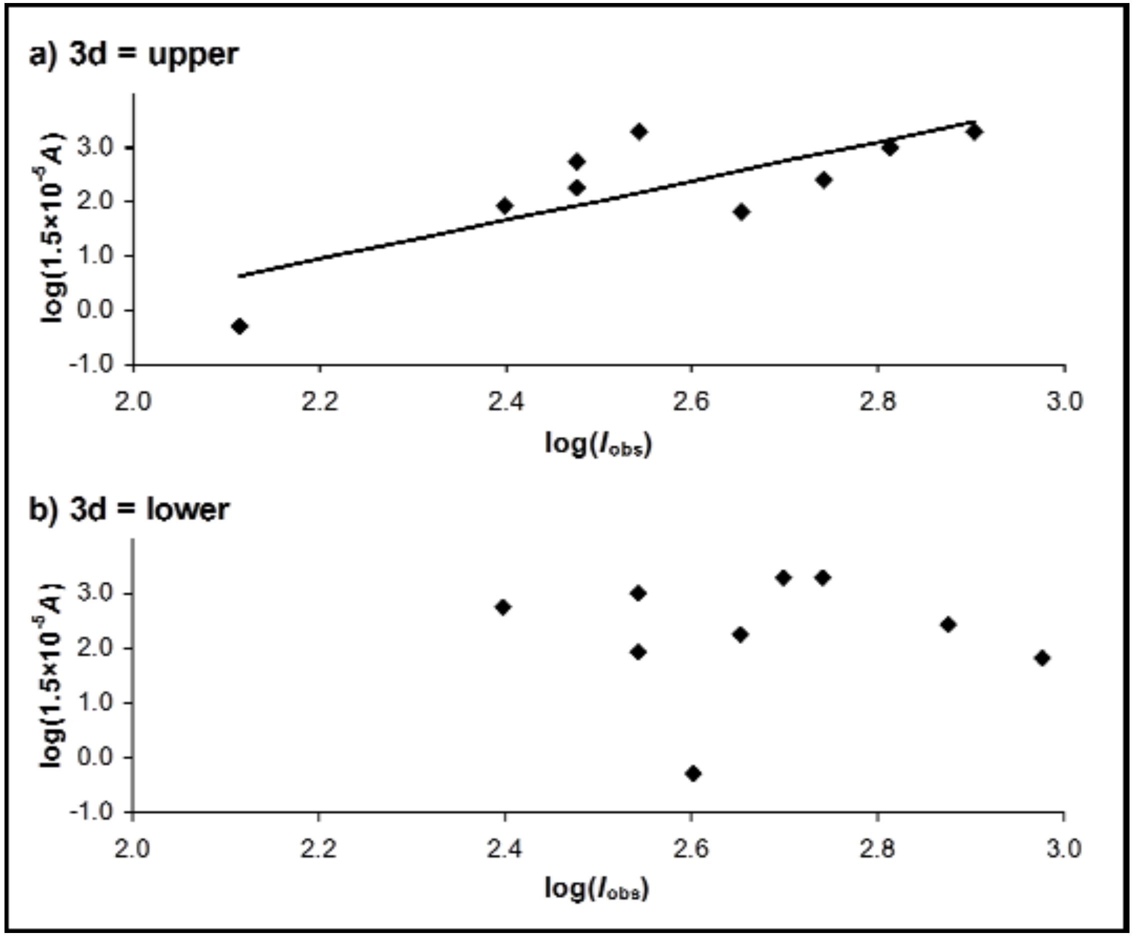
1. Introduction

Spectral lines are often characterized by their wavelength and intensity. The line intensity is a source-dependent quantity, but it is related to an atomic constant, the transition select the most accurate results, and to provide estimates of the uncertainties of the selected reference data.

At NIST we have critically evaluated transition probabilities and compiled tables of reference data for more than 30 years [1–4]. We have developed, and gradually refined, a system of data assessment, which is – in addition to general assessments of the various approaches – based on the following four main criteria:

1. Consideration of the critical factors of a method by the authors (as discussed below).
2. The authors' estimates of the uncertainty of their measured or calculated data.
3. The degree of agreement with other reliable data, based on tabular or graphical comparisons.
4. The fit of the data into systematic trends, or deviations from them.

Use of comparison of observed intensities and calculated *A*-values for level identification



Two *J*=1 levels in Na II:
$2p^5$**3d** $^3D°_1$ and $2p^5$**4s** $^1P°_1$:

333107.74 cm^{-1} and
333162.94 cm^{-1}

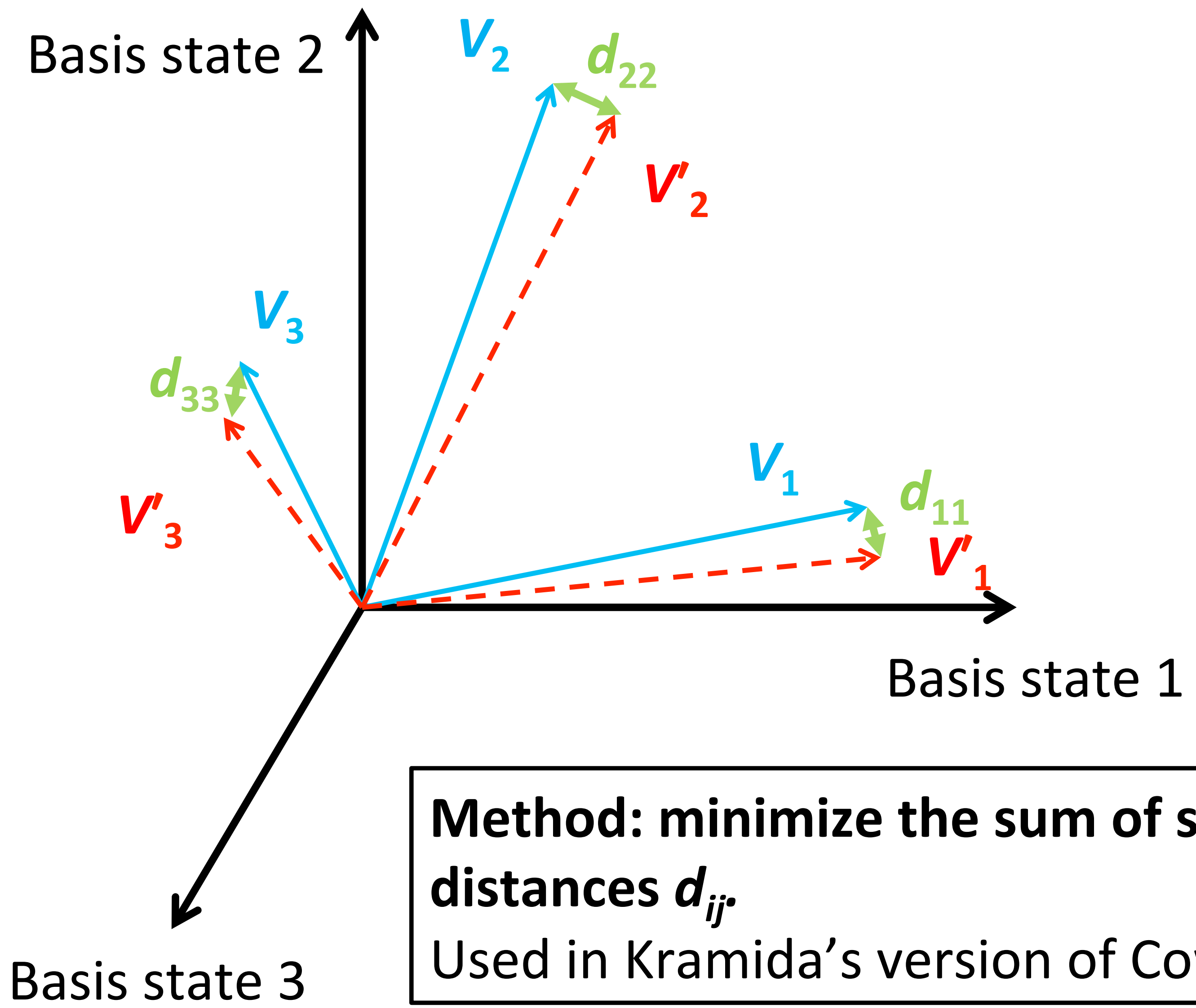
Which is which?

Result:
333162.94 cm^{-1} = **3d** $^3D°_1$
333107.74 cm^{-1} = **4s** $^1P°_1$

Identification in Wu 1971 is incorrect!

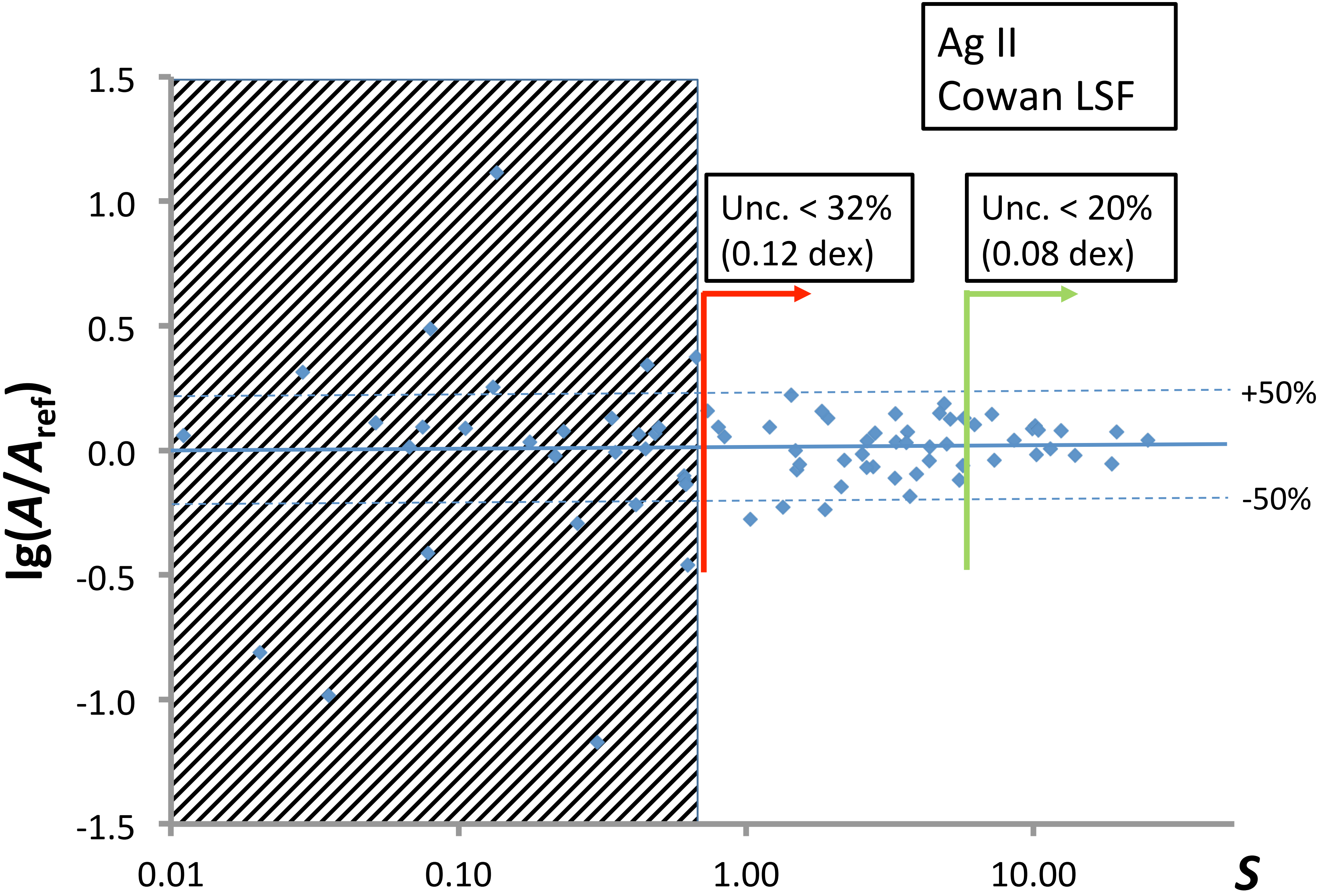
TP data from A. Hibbert et al., ADNDT **53**, 23 (1993)

Establishing correspondence between eigenvectors produced by two different atomic models



Method: minimize the sum of squares of distances d_{ij}.
Used in Kramida's version of Cowan's RCE.

Selection of *A* values based on line strength *S*

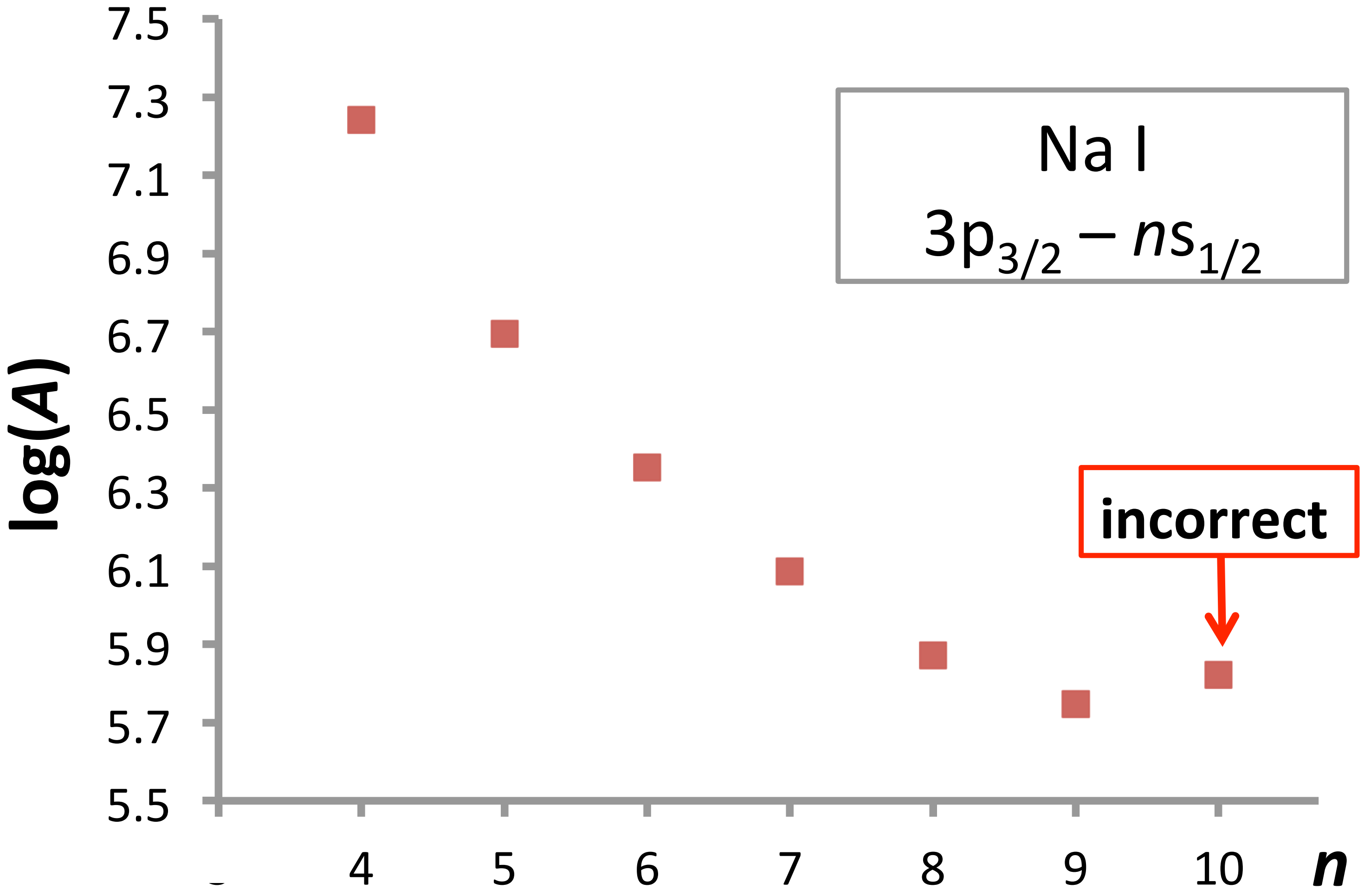


Cancellation Factor

$$CF = (S^+ - S^-)/(S^+ + S^-)$$

Values with $|CF| < 0.1$ are unreliable

Checking for regularities



TP data from Froese Fischer et al., ADNDT **92**, 607 (2006)

General conclusions

- Everything is doable in data evaluation:
  for every problem, there is a good recipe

- One unsolved problem: lack of workforce

Thank you for your attention!