R-matrix calculations along iso-electronic sequences

Michael Witthoeft, Allan Whiteford, Nigel Badnell

University of Strathclyde

Introduction

- Create a baseline data set for electron-impact excitation which is a step above distorted wave
- First sequence is F-like from Ne^{+} to Kr^{27+}
- Other priorities are: H-, He-, Li-, O-, and Ne-like sequences
- R-matrix script is used to simplify the process
- Analysis tools have been developed to handle the large amount of data

R-matrix Script

- A flexible Perl script to automate an R-matrix calculation
- works for serial or parallel machines
- calculation sequence:
    - AUTOSCTRUCTURE (structure and high-energy limit points)
    - ICFT R-matrix calculation
    - produce adf04 file (fully commented)
- supports radiation damping
- no Auger damping yet

R-matrix Analysis Package (RAP)

RAP base package:

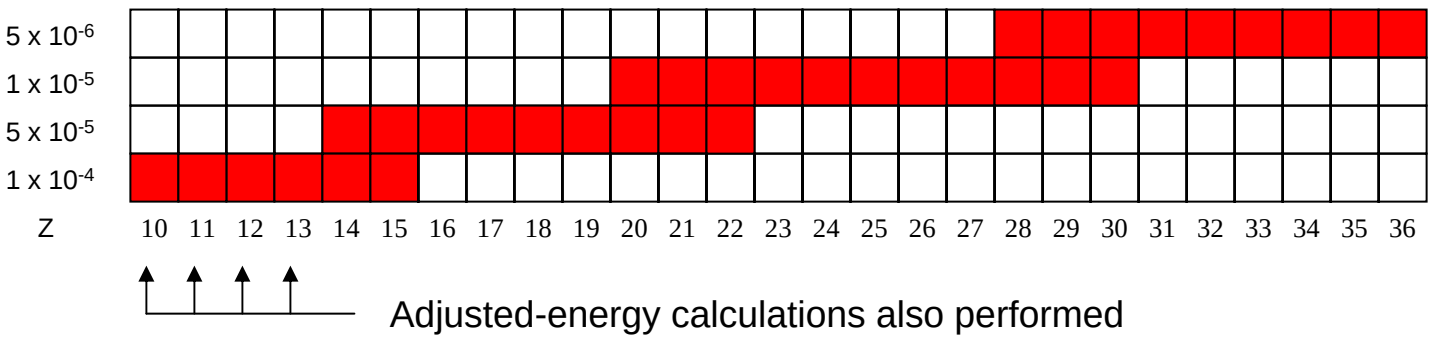
- a set of Python routines that read and manipulate the R-matrix results
- reads in:
    - adf04 files
    - AUTOSTRUCTURE output files (GF values)
    - TCCDW.DAT files (term coupling coefficients)

RAP GUI:

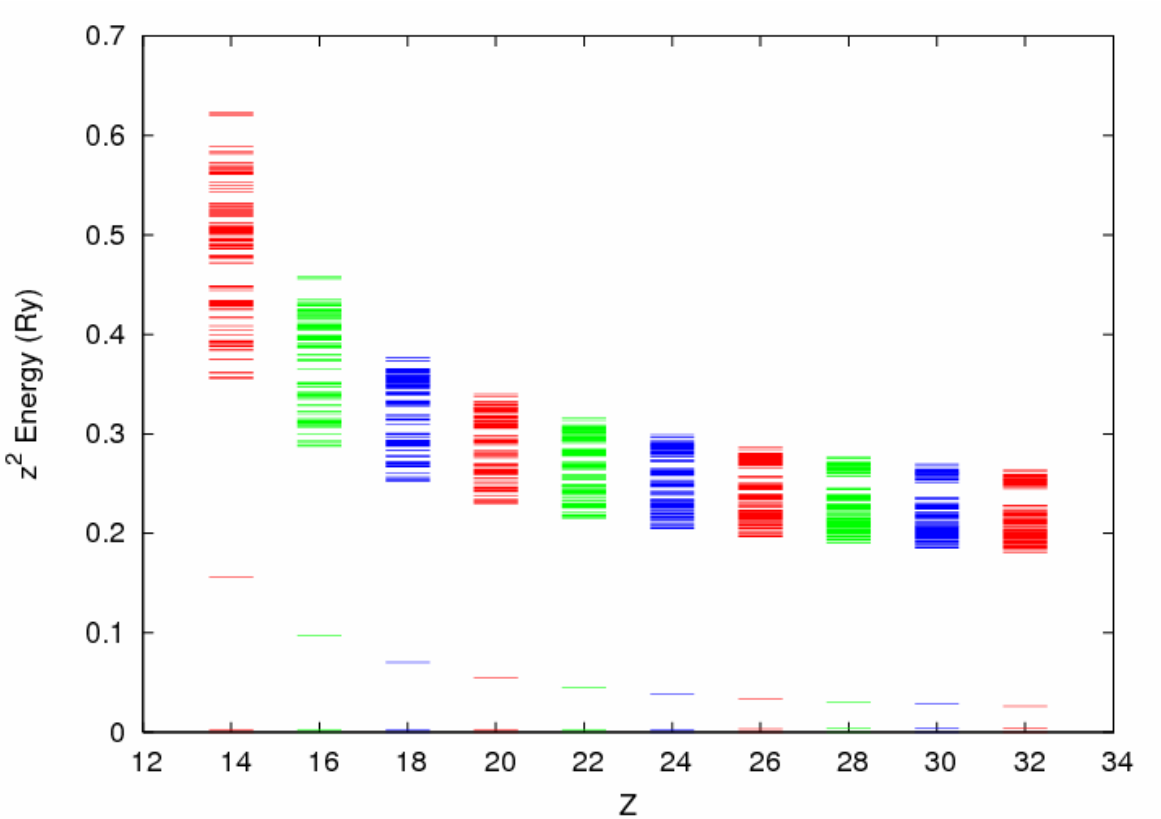
- Graphical interface to the routines in the base package
- Produce data files and plots of energies and effective collision strengths

F-like Sequence

- ICFT calculation with 87 terms and 195 levels.
- contains the configurations
  - $2s^2\ 2p^5$ (two fine-structure levels)
  - $2s\ 2p^6$
  - $2s^2\ 2p^4\ 3l$
  - $2s\ 2p^5\ 3l$
  - $2s^2\ 2p^4\ 4l$
- Scaling parameters for the structure are optimized for each individual ion.
- All ions from Ne^+ to Kr^{27+}



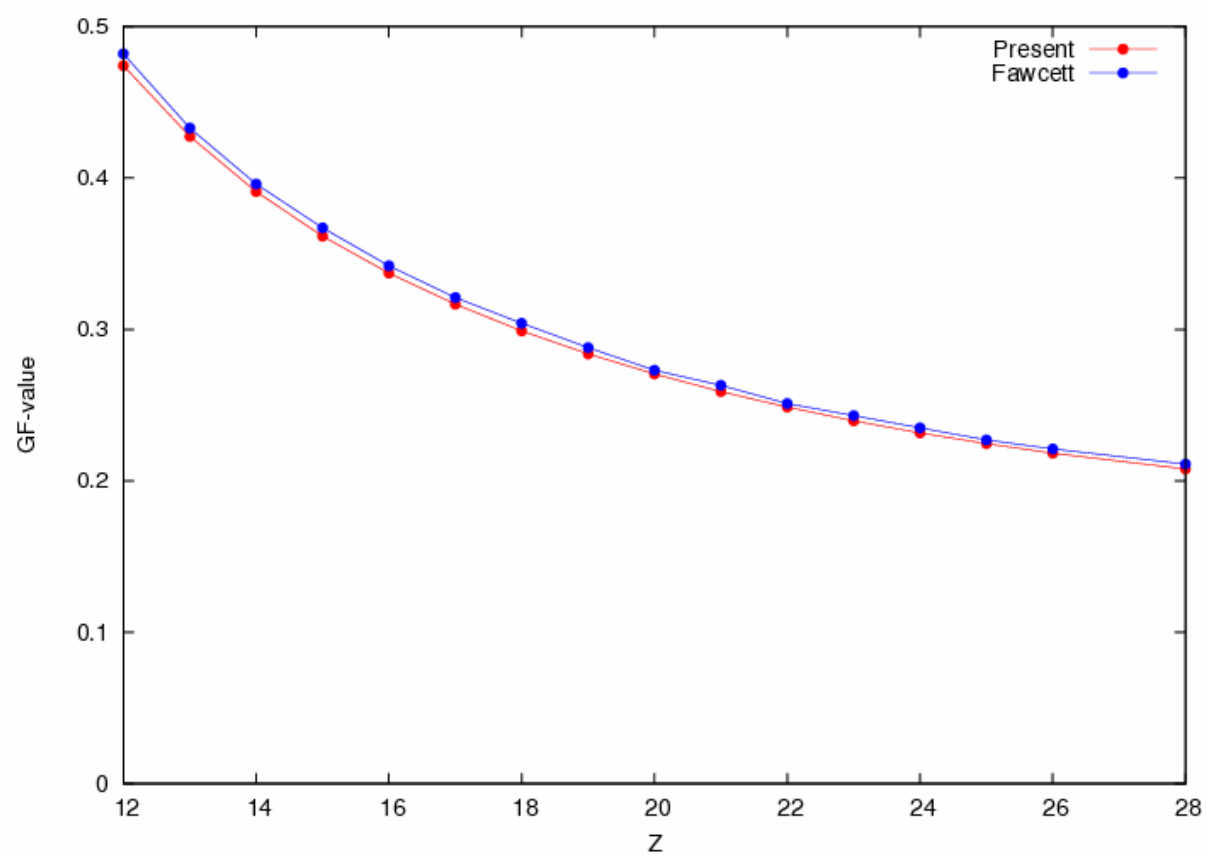
Structure



A look at the energy level distribution for several ions along the sequence. Note the gap forming between the n=3 and n=4 levels as Z increases. We also see that the energies scale as z^2 for the higher charges.

Structure

gf-values are also a useful metric for determining the quality of the structure. Here we compare to values calculated by Fawcett (1984) using relativistic Hartree-Fock theory. For this transition, we see excellent agreement along the entire sequence.

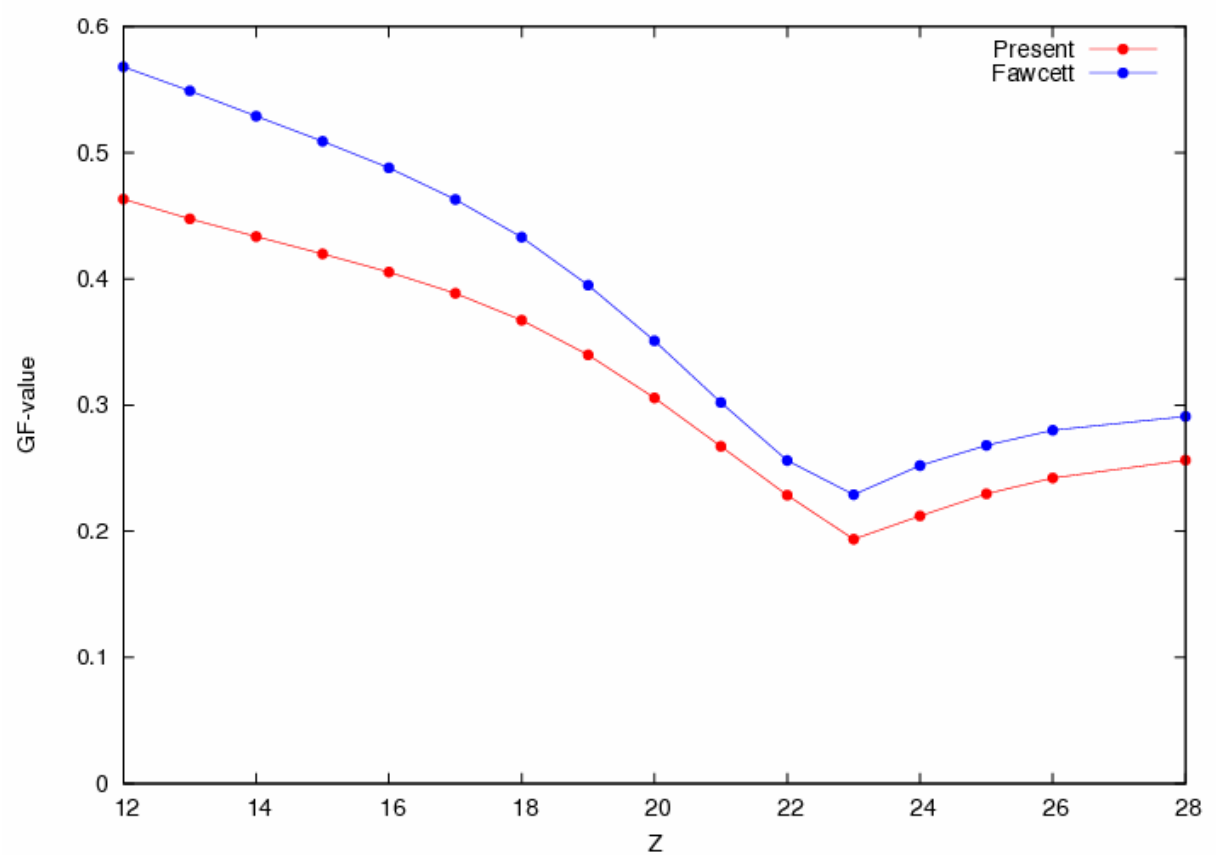


Fawcett, ADNDT **31**, 495 (1984)

Structure

We see a larger difference between the calculations for this 3s transition, but still has good general agreement.

$2s^2\ 2p^5\ {}^2P_{3/2} - 2s^2\ 2p^4\ 3s\ {}^2P_{3/2}$

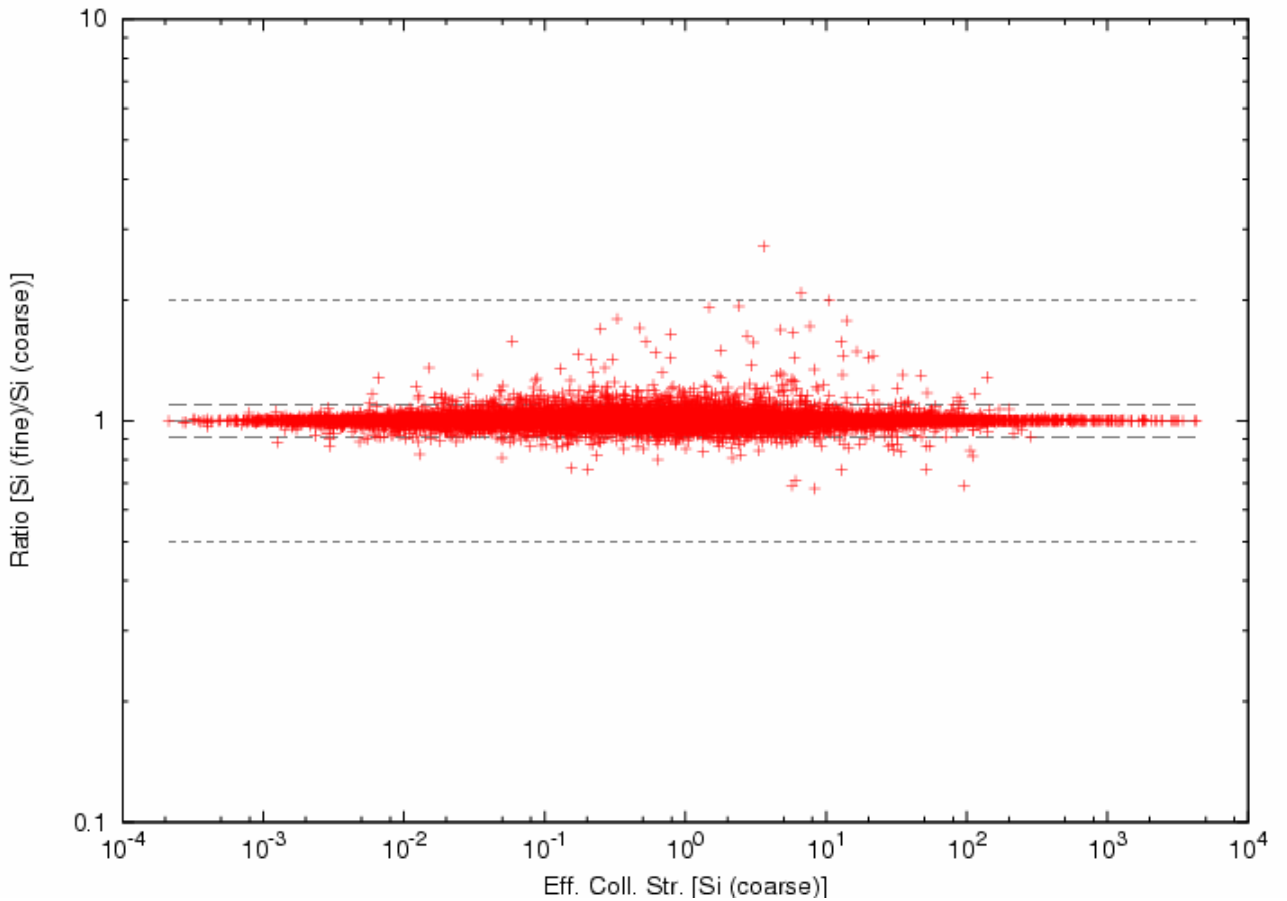


Energy mesh convergence

First overlap region: Si^{5+} and P^{6+} for 10^{-4} and $5x10^{-5}$ z^2 Ry meshes

A useful tool to explore differences between two calculations for all the transitions is the scatter plot. The plot below is for Si^{5+} at a temperature of $7.2x10^4$ K.

The advantage of these plots is that large differences pop out. Note: only 2.5% of the transitions disagree by more than 10% at this temperature.



Comparisons

Excitation calculations have been done for a number of ions along the F-like sequence. Work before 1994 has been comprehensively reviewed by A. K. Bhatia. Mohan et al. performed LS R-matrix calculations, in a series of papers, for many ions along the sequence (Mg^{3+}, Si^{5+}, S^{7+}, Cl^{8+}, Ti^{13+}, Fe^{17+}, and Ni^{19+})

Our main comparisons will be with:

- fine-structure transition over the sequence (Saraph & Tully, 1994, Berrington et al., 1998)
- Ne^{+} (Griffin et al., 2001)
- Fe^{17+} (Witthoeft et al., 2006)

Saraph & Tully, A&A 107, **29** (1994)

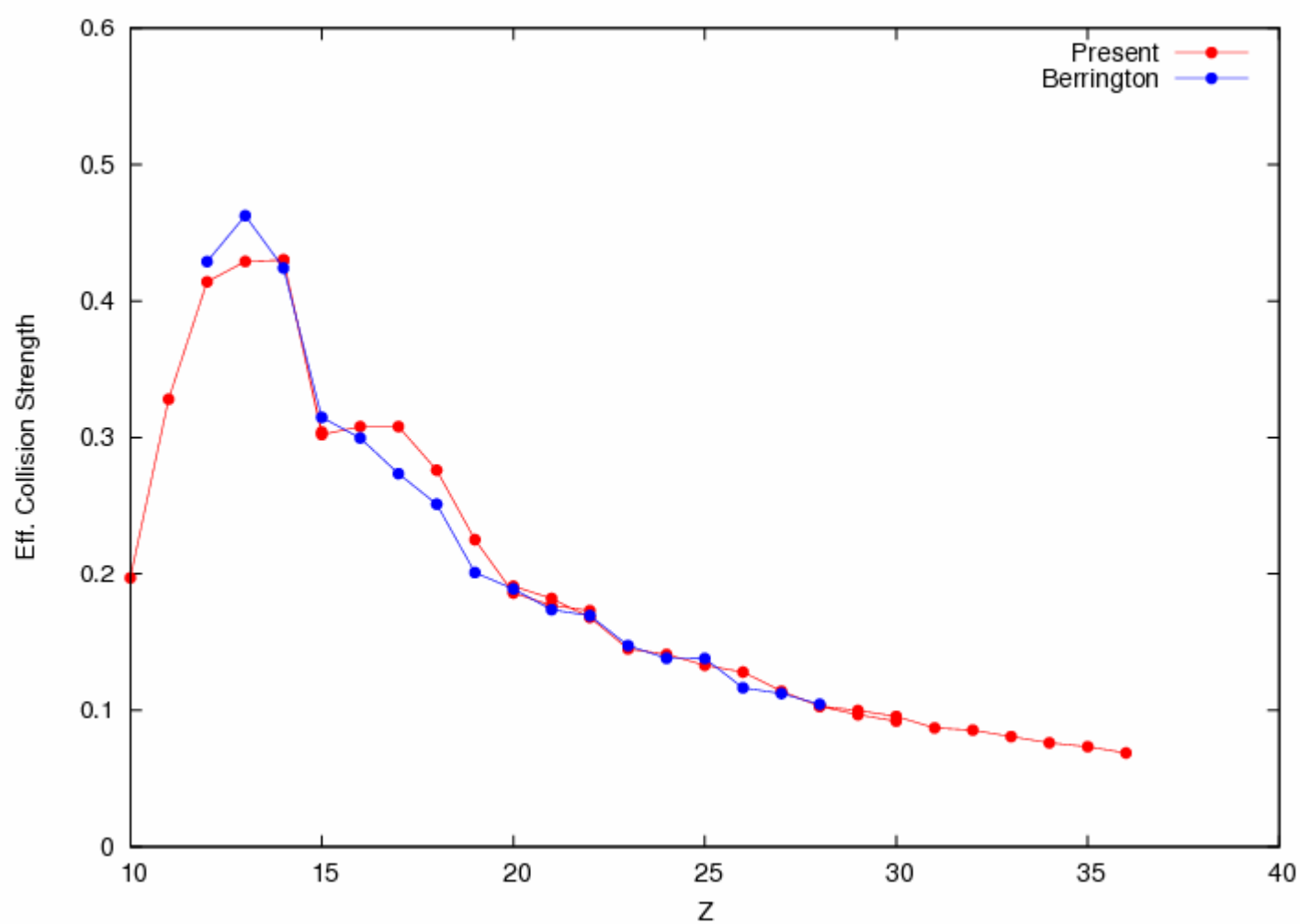
Bhatia, ADNDT **57**, 253 (1994)

Griffin et al., JPB **34**, 4401 (2001)

Witthoeft et al., A&A **446**, 361 (2006)

Fine-structure

$T = 10^4 z^2$ K



Fine-structure

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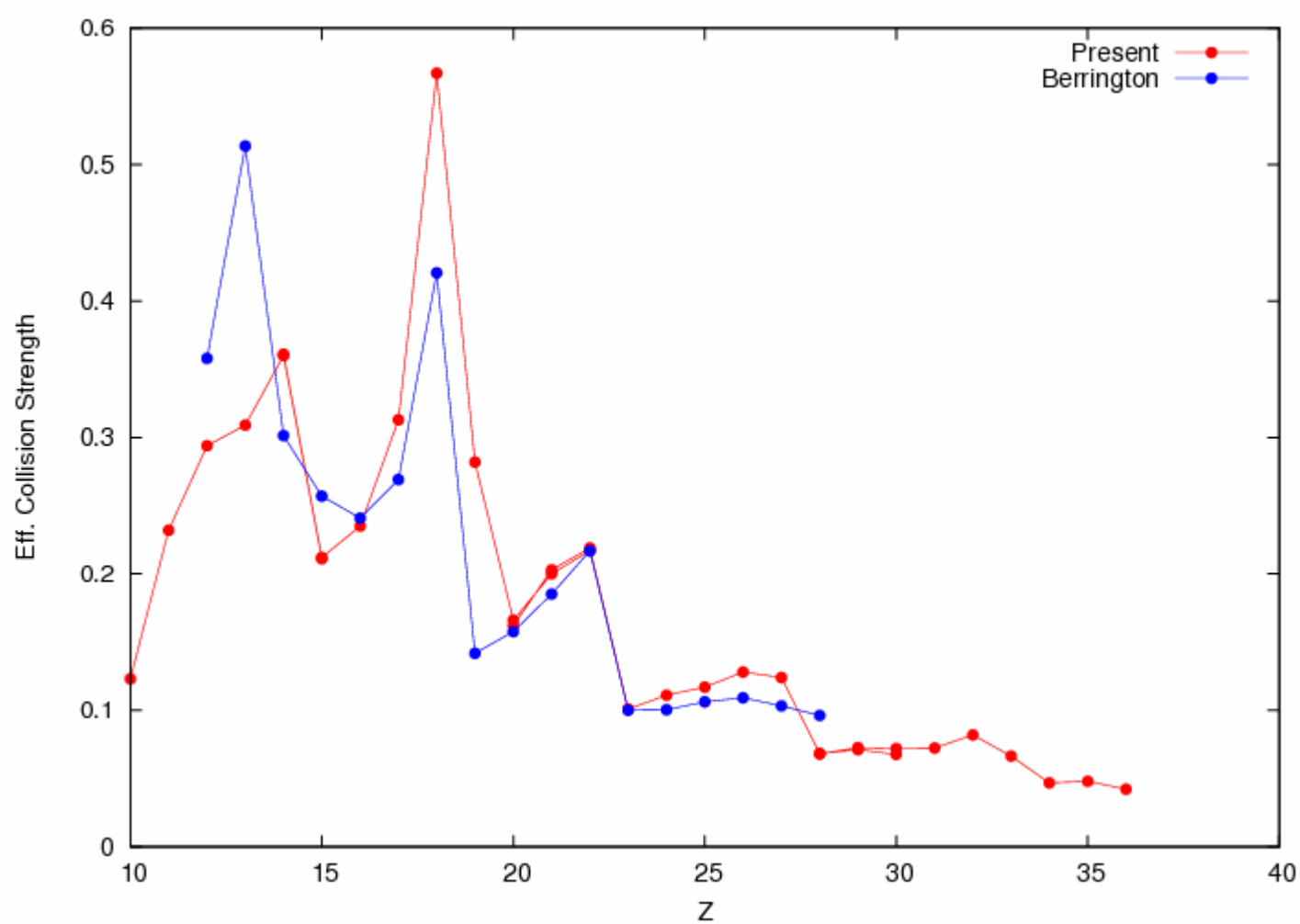


F-like Fe

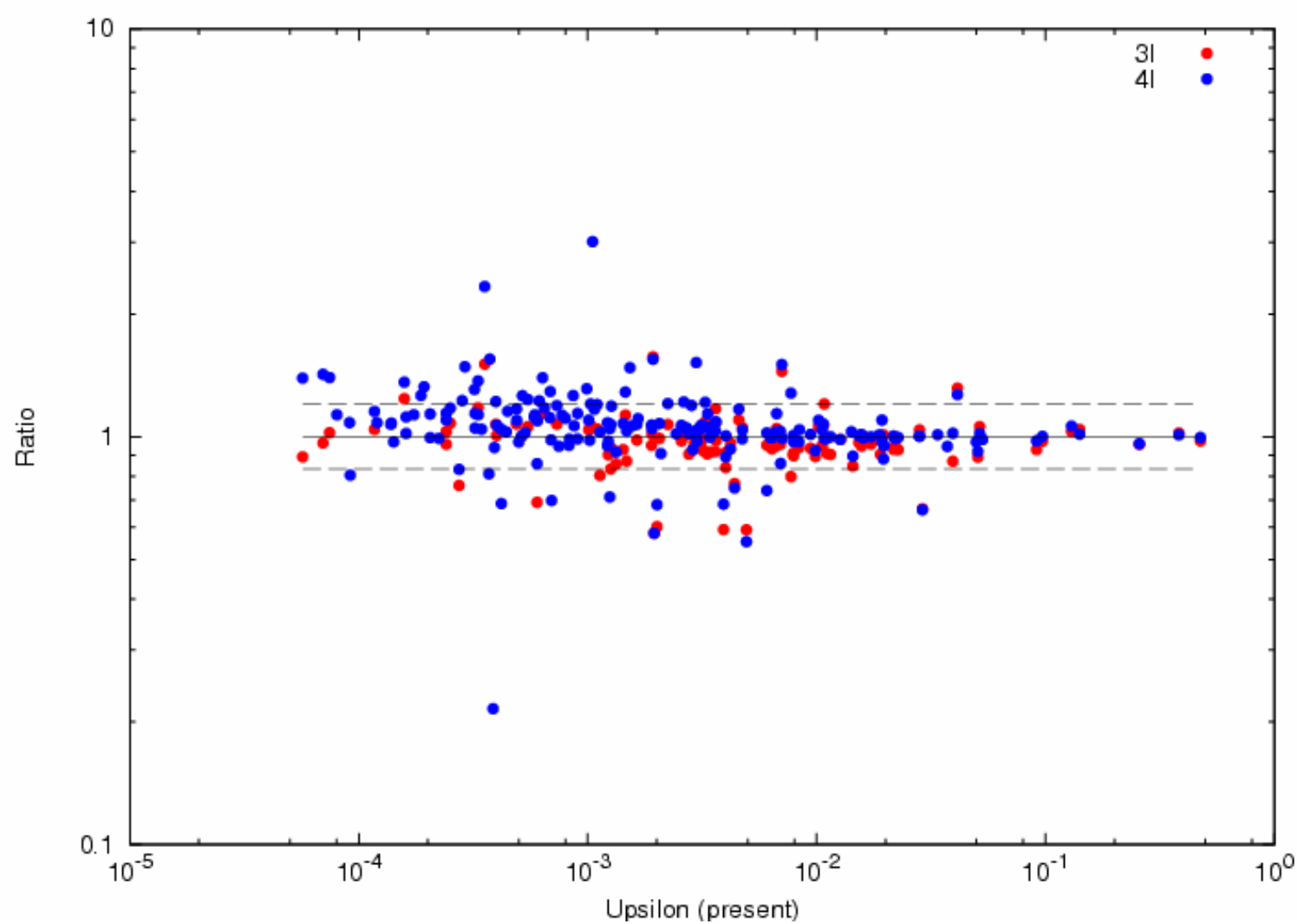
Compare the F-like Fe calculation with a recent calculation by Witthoeft et al. (2006). The previous work consists of two calculations; one with an n=3 target expansion and the other up to n=4.

conf.	old n=3	old n=4	new
2s2 2p5	✓	✓	✓
2s 2p6	✓	✓	✓
2s2 2p4 3l	✓	✓	✓
2s 2p5 3l	✓	✓	✓
2p6 3l	✓	✓	
2s2 2p4 4l		✓	✓
2s 2p5 4l		✓	
2p6 4l		✓	

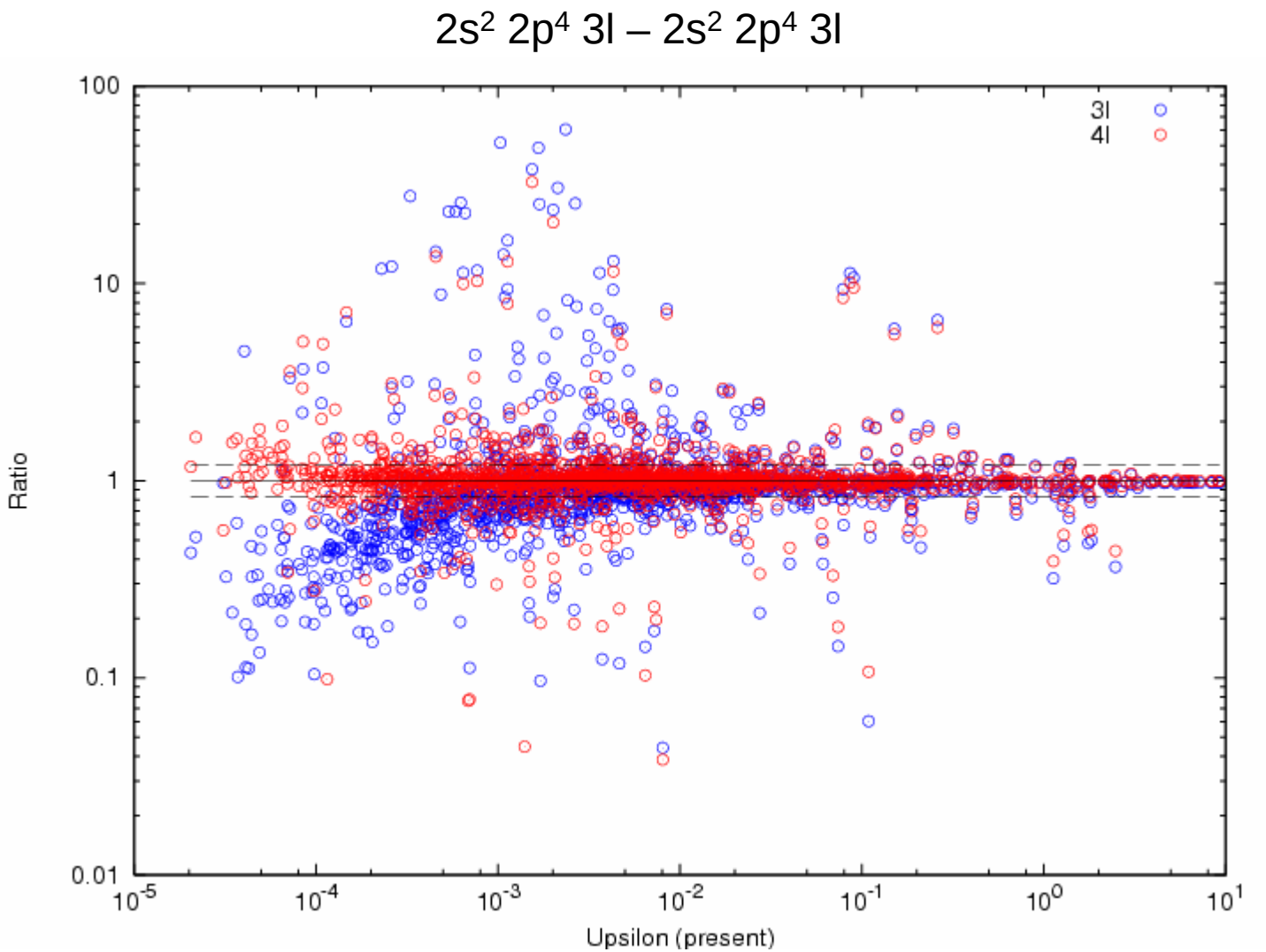
Witthoeft et al., A&A **446**, 361 (2006)

F-like Fe

Transitions from the ground level:

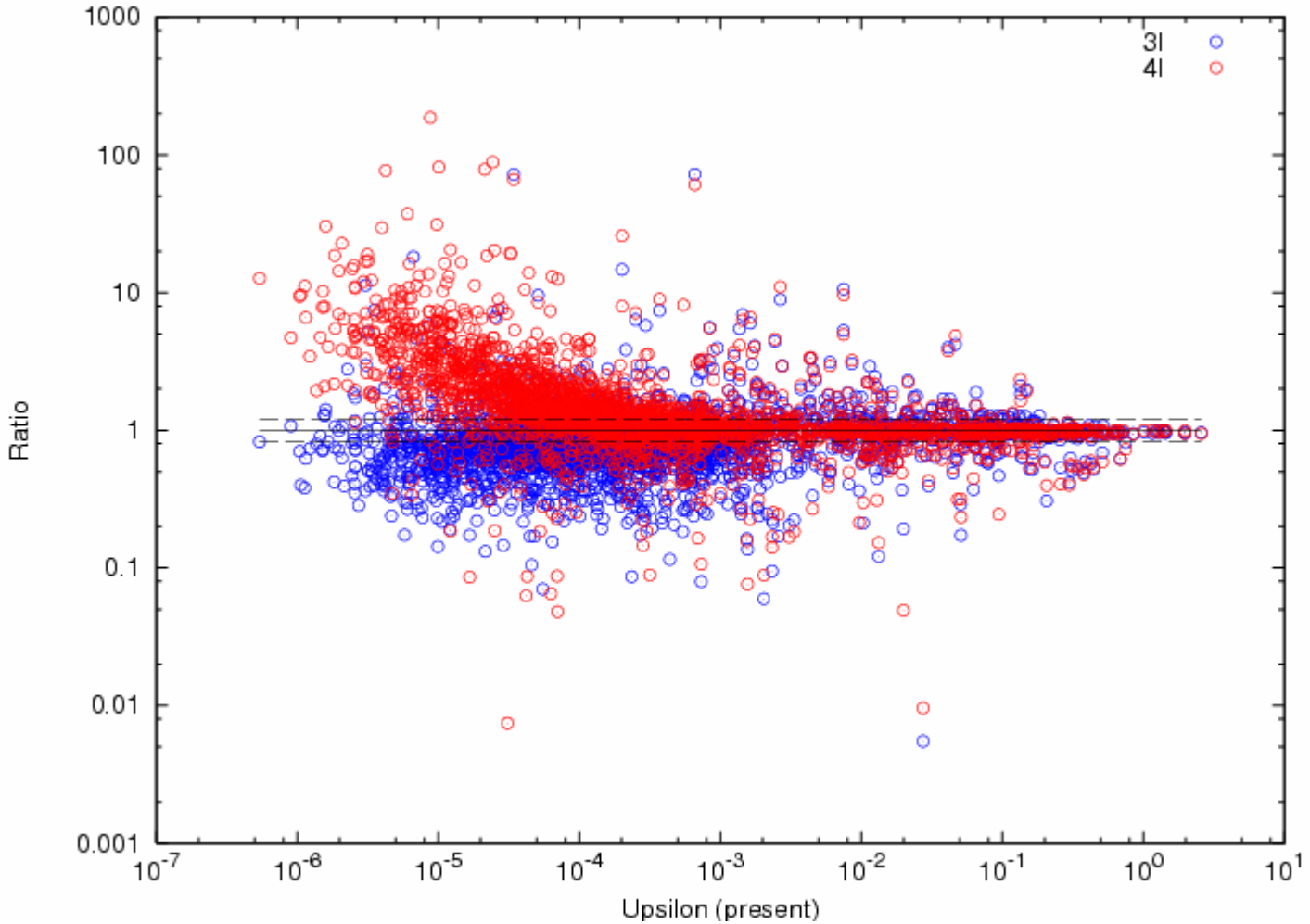


F-like Fe

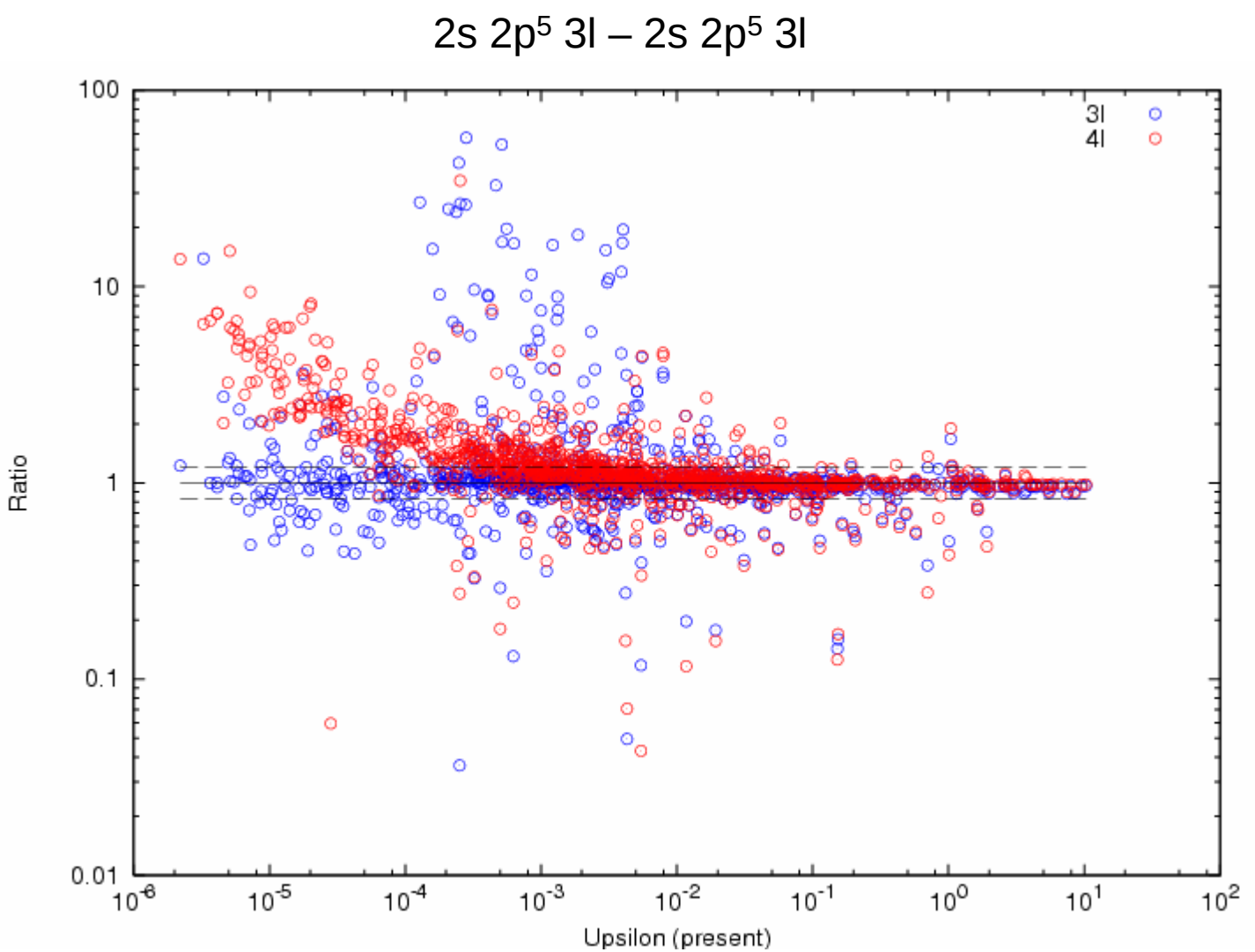

2s² 2p⁴ 3l – 2s² 2p⁴ 3l
3l
4l
Ratio
Upsilon (present)
100
10
1
0.1
0.01
10⁻⁵
10⁻⁴
10⁻³
10⁻²
10⁻¹
10⁰
10¹

F-like Fe

$2s^2\ 2p^4\ 3l - 2s\ 2p^5\ 3l$



F-like Fe


2s 2p5 3l – 2s 2p5 3l
100
10
1
0.1
0.01
Ratio
3l
4l
10-6
10-5
10-4
10-3
10-2
10-1
100
101
102
Upsilon (present)