R-matrix as part of the fundamental atomic structure and collisional data required for Tungsten ions.

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Preparatory Consultancy Meeting for the Tungsten Ions CRP

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- ***The Mandate:***
  - Address the data needs in the area of the ionization balance and spectroscopic and collisional properties of tungsten at temperatures between 1keV and 10keV which are currently subject to large uncertainties and disagreements between theory and experiment.

  - Ionization balance = ground and metastable ionization vrs recombination (RR and DR).
  - Metastable ionization => implies knowing the population of excited states=> electron-impact excitation. However, for highly charged systems, the number of 'metastables' reduces → gs to gs.

Various tungsten ionization fraction curves from Thomas Putterich, Stuart Loch, Simon Preval and Nigel Badnell

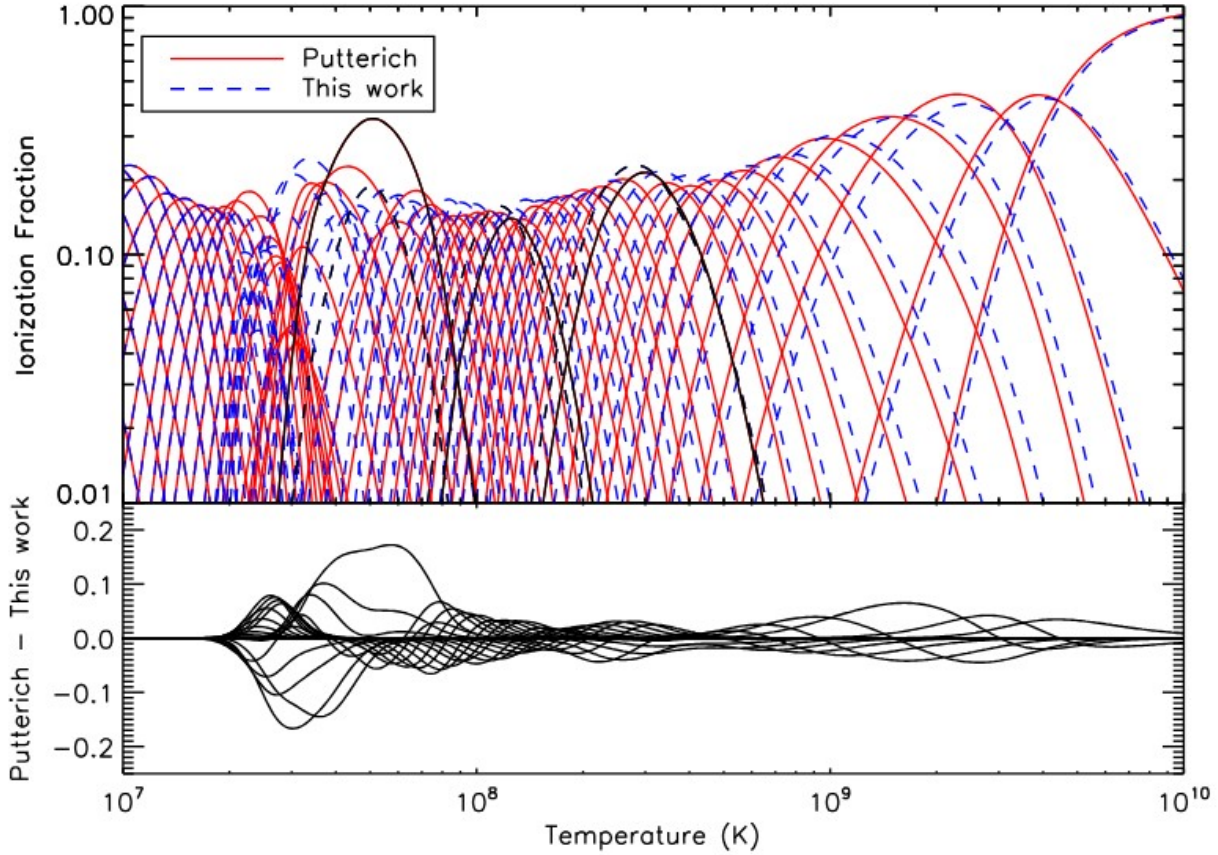

Figure 29. Tungsten ionization fraction using Pütterich *et al* 's [12] recombination rate coefficients (solid) and our recombination rate coefficients (dashed) up to 36-like. Both ionization fractions use the ionization rate coefficients of Loch *et al* [14]. From left to right, we have marked the fractions of 28-like, 18-like, and 10-like in black. The bottom plot shows the difference between Pütterich *et al* 's and our ionization fraction.

between 1keV and 10keV, is approximately 10^7 -10^8 Kelvin.

You might consider Ni-like W as a potential dividing line where excited state ionization becomes less important.

However, there are approx. 20 ion stages > 10 ^7 K , yet before Ni-like W (ie. 3d^10)

These 20 ion stages are theoretically difficult to converge, let alone know accurately. They involve half-open d and f shell systems. Even NIST/experiment has only a limited number of known levels for certain ion stages.

NIST Atomic Spectra Database Levels Data

Example o
Kramida, A.
Spectra Da
[2024, Aug
Gaithersbu

W XXXII 4 Levels Found

***Z* = 74, Tc isoelectronic sequence**

Data on Landé factors are not available for this ion in ASD

Primary data source	Query NIST Bibliographic Database for **W XXXII** (new window)
Kramida and Shirai 2009	Literature on W XXXII Energy Levels

Configuration	Term	J	Level (Ry)	Uncertainty (Ry)	Leading percentages			Reference
$4d^7$	^{4}F	$^9/_2$	0.00000	0	63	31	^{2}G	L14671
		$^7/_2$	1.1322	0.0004	87	11	^{2}G	L12340c24
$4d^7$	^{2}H	$^9/_2$	1.3667	0.0004	35	33	^{2}G	L12340c24
W XXXIII ($4d^6$ $^5D_4$)	**Limit**	**---**	**[94.33]**	**0.10**				**L9087**

If you did not find the data you need, please inform the ASD Team.

Low lying levels are very highly mixed, the unknown excited states will be more so!

Even for simpler systems (Be-like Al), dipole transitions within the n=2 complex converge very well, but dipole transitions from n=2 to n=4 vary between a CI expansion of 98 levels vrs 238 ! (Fernandez-Menchero) MNRAS 450, 4174–4183 (2015)

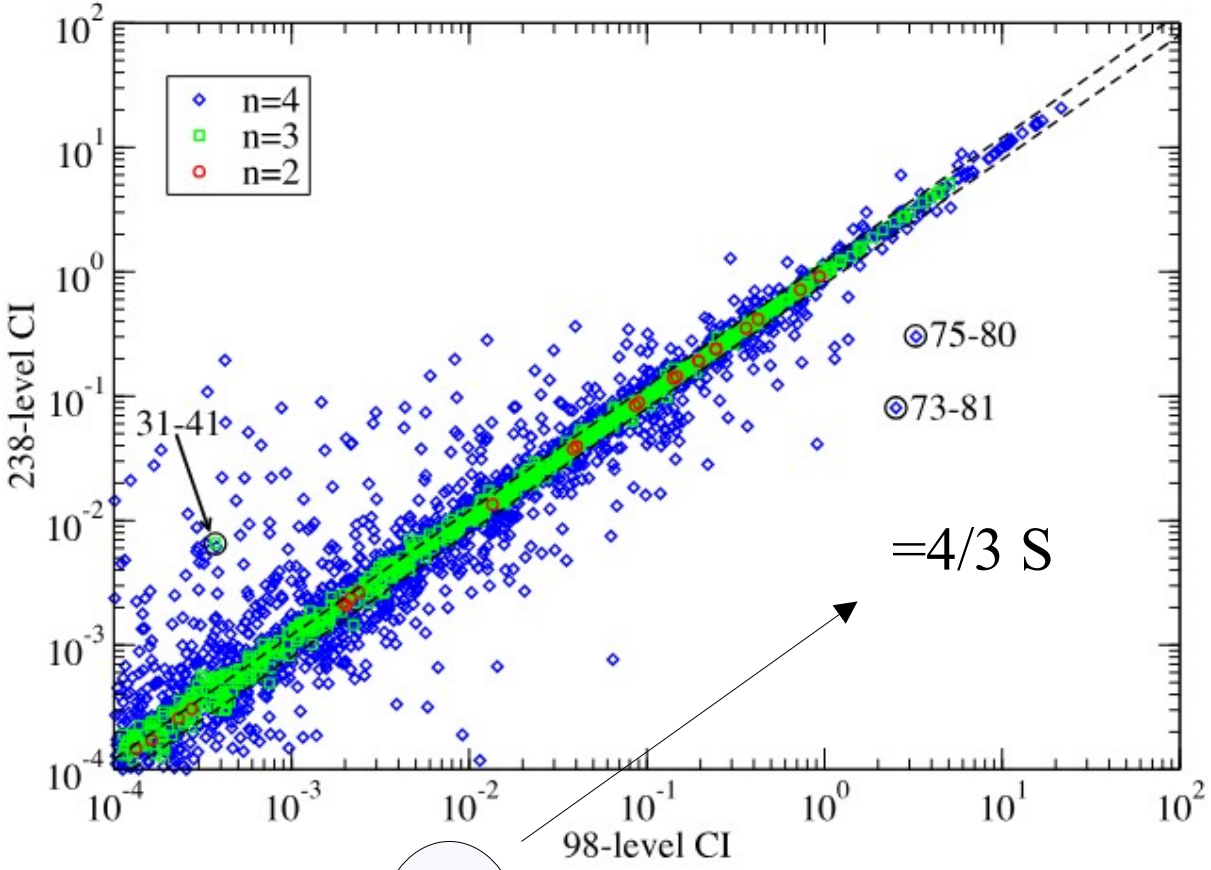

Figure 1. A comparison of y_∞ (see equation 4) for the 98- versus 238-level CI atomic structures for transitions amongst the 98 lowest common levels of Al $^{9+}$. ○: transitions with upper level with $n = 2$; □: transitions with upper level with $n = 3$; ◇: transitions with upper level with $n = 4$; dashed lines: 20 per cent fractional difference.

(1)The question becomes, why would we theoretically expect the excited states of W^(26+)-W^(45+) to have converged in terms of energies or A-values?

(2)Follow-on question: how do the transitions between these excited of tungsten effect the total radiative power at certain temperatures and densities ?

Perhaps, identifying transitions regardless of their accuracy that contribute to the total power is a way forward? foreshadow

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- I hope that I have argued that theoretical spectroscopic prediction without some experimental calibration is very challenging (but perhaps EBIT experiments could provide some valuable wavelength accuracy)
- Collisional work it built upon the atomic structure (ie. GRASP0,GRASP2018,AUTOSTRUCTURE,HULLAC,FAC) but is only as good as the target.

- ***ADAS :Stuart Henderson, Martin O'Mullane and Nigel Badnell.***
- ***Take W^(31+) : [1] 4s2 4p6 4d7, 4s2 4p5 4d8,4s2 4p6 4d6 4f***

(groundstate and first two metastable configurations)

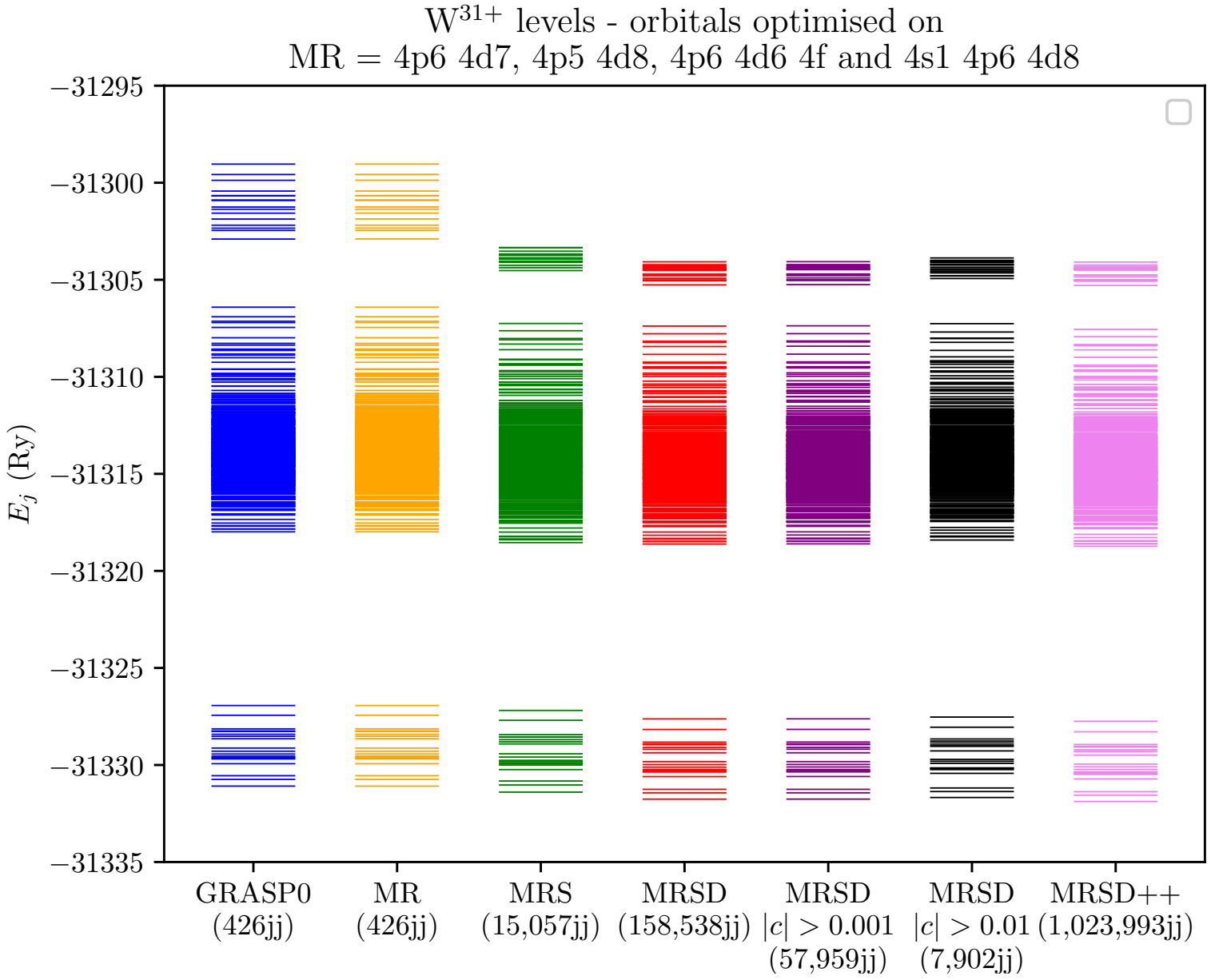
[2] create list of excited configurations using these three 'base configurations' … ie involving single and double promotions

[3] Using the ionization balance curves or otherwise choose and appropriate density and temperature before a CONFIGURATION AVERAGE distorted wave to work out CA excited state populations

[4] Using a threshold value, throw away configurations with small populations that do not contribute to the total power loss.

[5] Refined level-resolved calculations with subset.

- ***QUB approach employing options with the GRASP2018 code of Prof P. Jonnson.***



- ‘uncertainties and disagreements between theory and experiment.’

→ atomic structure : free-electron laser +EBIT experiments
to ‘dial-in’ a transition wavelength and
measure A-value (Fe16+ £C/3D)

→ University plasma devices suffer from significant impurity elements as well as Tungsten/Molybdenum, and high chance of blended lines.

→ others have greater experience in this area.