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The Tungsten Project: Electron-ion recombination rate coefficients for the isonuclear sequence of tungsten

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Outline

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- Motivation - ITER
- The Tungsten Project
- Calculation Methods
- Results and Comparisons
- Conclusion

Motivation & Aims

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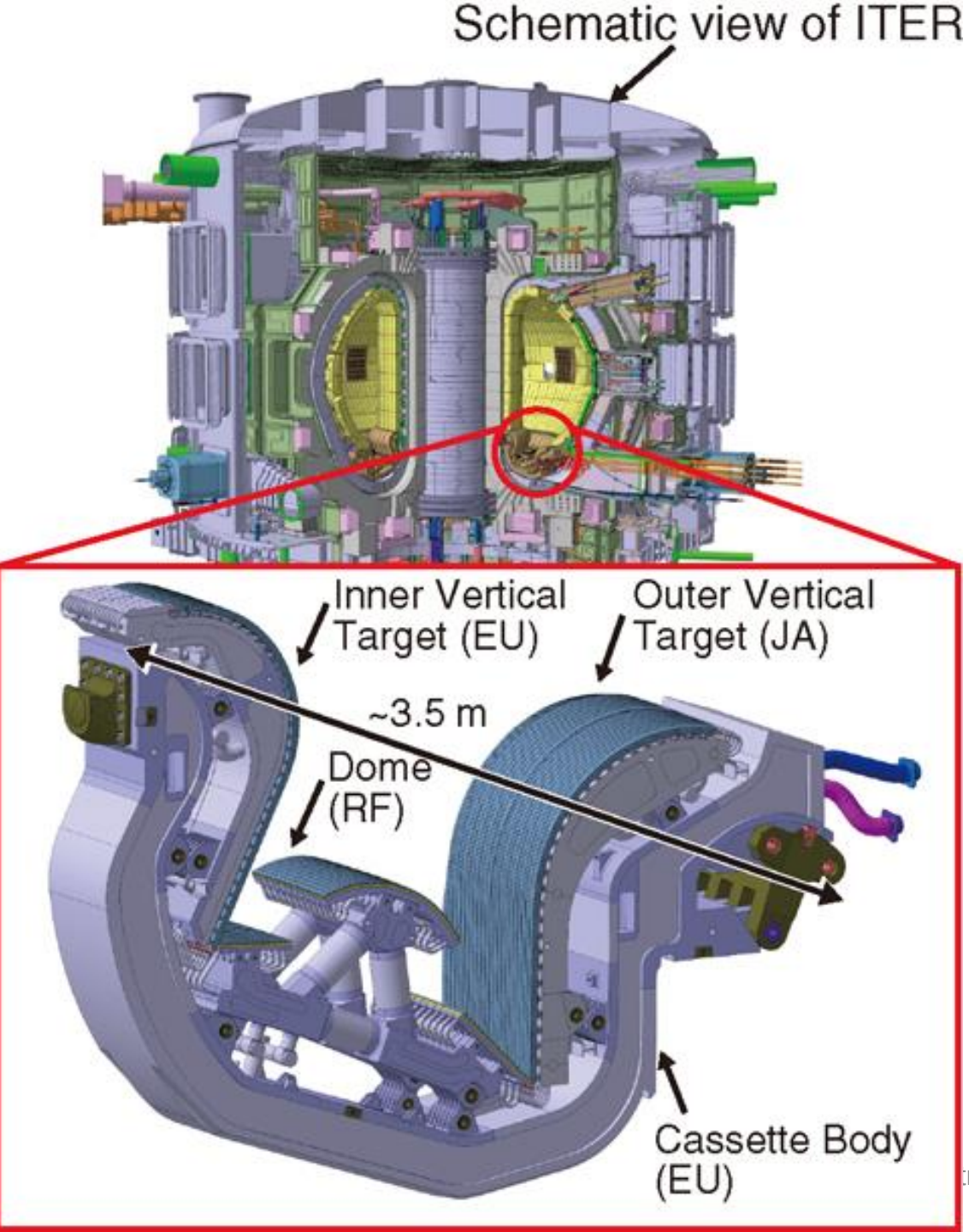
- ITER nuclear fusion reactor currently being built in Cadarache, France.
- First plasma projected for 2025.
- Dwarfs Joint European Torus (JET) in terms of plasma volume and reactor size.
- Aims to generate energy with Q=10 (output energy 10 times the input).



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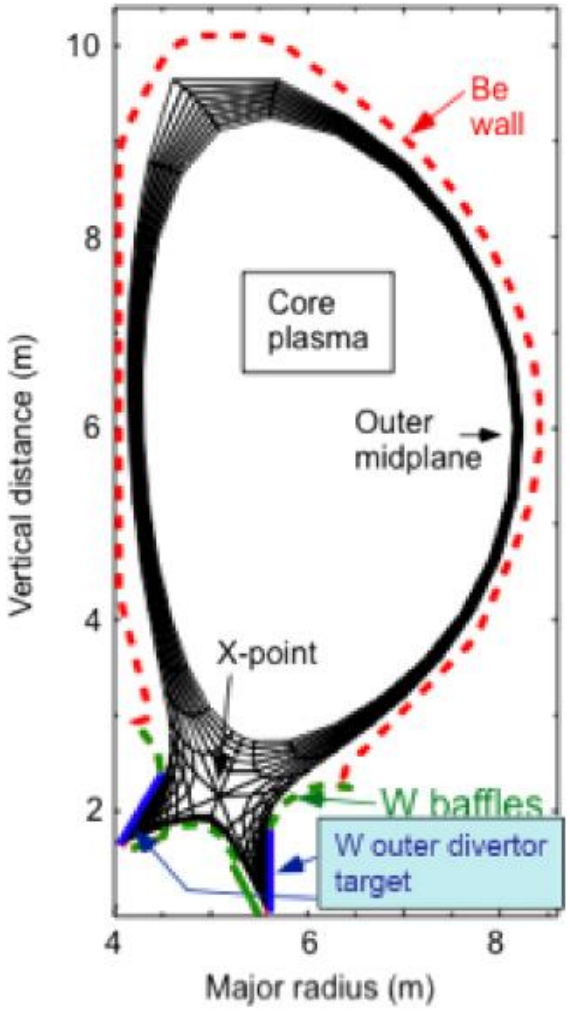

tralia

Motivation & Aims

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- The divertor will be composed of tungsten. Why?
  - Tungsten has high melting point.
  - Low affinity for tritium absorption.
  - Can withstand large power loads.
- Plasma will occasionally make contact with the divertor, sputtering tungsten impurities into the core plasma.

Motivation & Aims

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- Heavy ions are very efficient radiators. Tungsten impurities will cool the plasma, and can potentially quench it.
- Detailed collisional-radiative (CR) modelling required to understand the effects of these impurities.
- Require complete, isonuclear DR rate coefficients for ion being modelled.

Background

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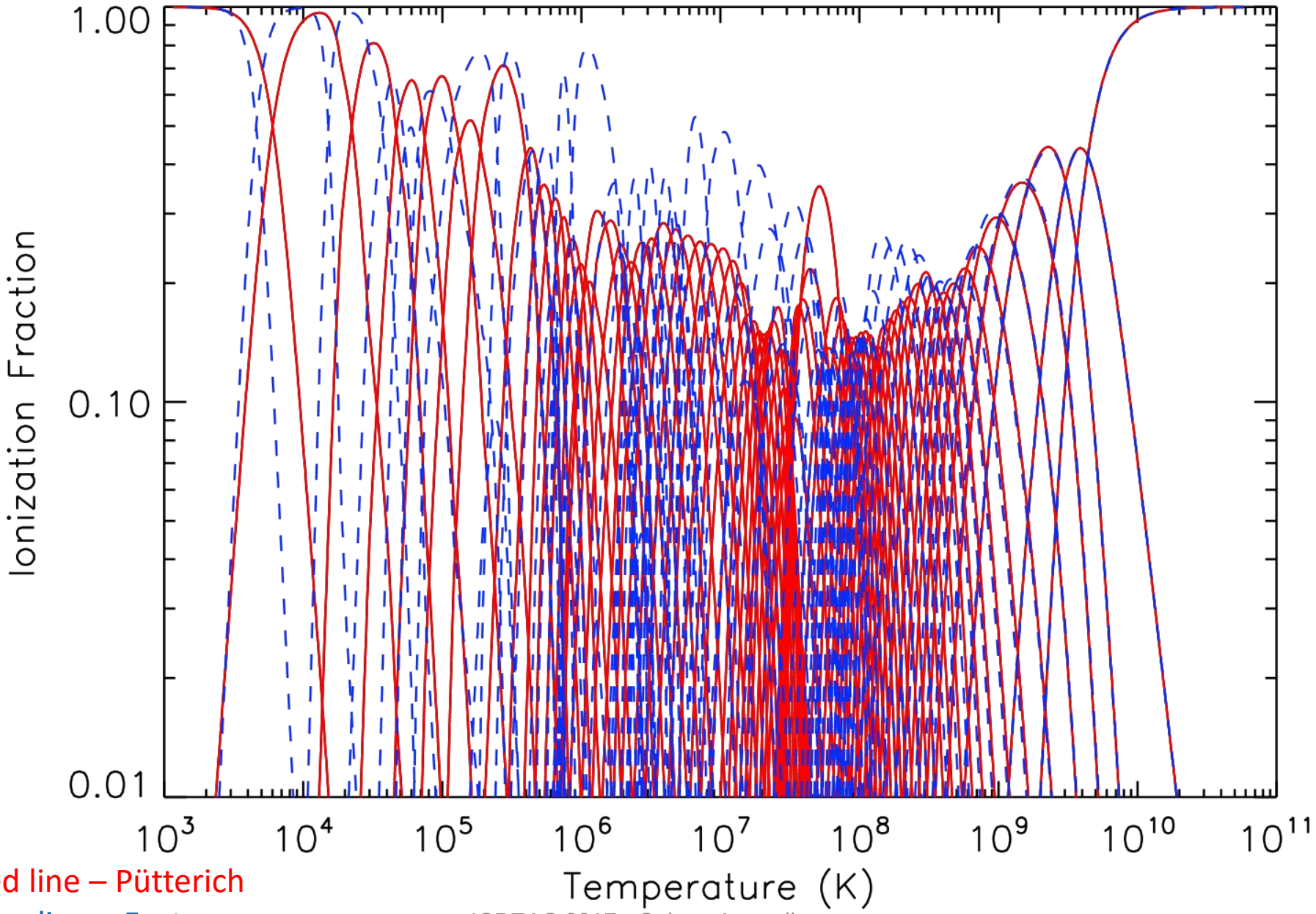
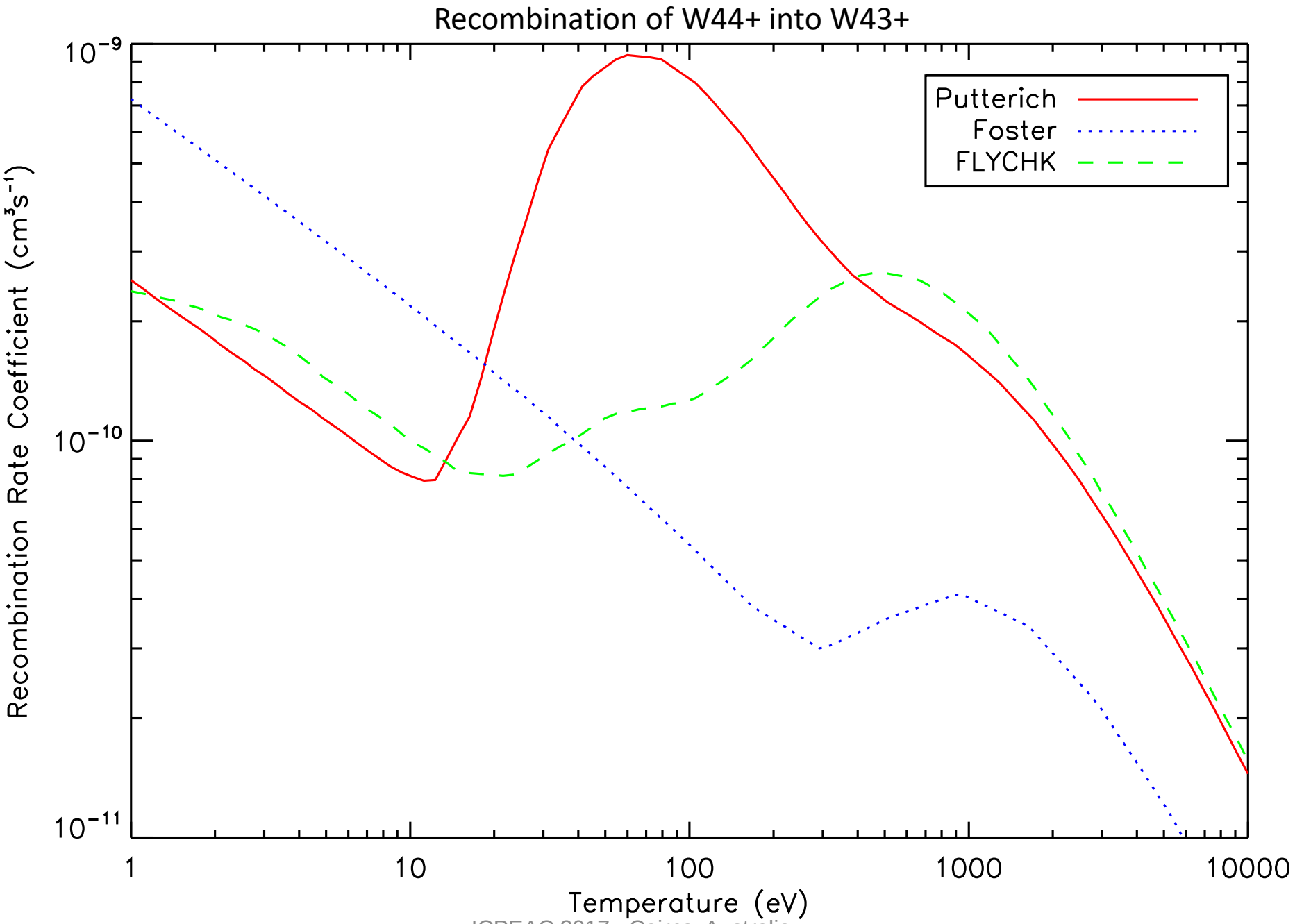
- Several Tungsten DR data sets exist:
  - Pütterich et al. (2008), empirically scaled ADPAK data (Post et al. 1977, 1995).
  - Foster (2008), Burgess General Formula.
  - Chung et al. (2005), FLYCHK.
- Compare steady-state ionization balances computed using ionization rate coefficients from Loch et al. (2005), and Pütterich/Foster DR rate coefficients.



Red line – Pütterich

Blue line – Foster


Recombination of W44+ into W43+
Putterich
Foster
FLYCHK
Recombination Rate Coefficient (cm³s⁻¹)
10⁻⁹
10⁻¹⁰
10⁻¹¹
1
10
100
1000
10000
Temperature (eV)

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- Created to calculate a set of self consistent, partial, final-state resolved DR rate coefficients for entire isonuclear sequence of Tungsten.
- Data hosted on OPEN-ADAS, calculated using AUTOSTRUCTURE (Badnell 1986, 1997, 2011).

The Tungsten Project

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- AUTOSTRUCTURE is a distorted wave code using kappa-averaged semi-relativistic wavefunctions calculated with a TFDA potential.
- Calculates level, term, or configuration resolved energies, radiative/autoionization rates, and many other atomic quantities.

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- It gets difficult remembering what comes after Z=30 on the periodic table…
- Instead of referring to an ion by the metal it represents (i.e. Zn-like), refer to these by their Z.
- E.g. Si-like is now 14-like, Zn-like is 30-like, and Gd-like (Gadolinium) is 64-like.

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- For 01- to 48-like ($4f^2$), DR rate coefficients are calculated in core excitations, labelled by initial and final principal quantum number n_i and n_f respectively.
- E.g. A core excitation beginning at $n_i = 3$ and finishing at $n_f = 4$ is $3 - 4$.
- We check if a core excitation is worth calculating in IC by looking at its contribution to the total in configuration average.

The Tungsten Project

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- Summing over autoionizing states, the Rydberg electron is calculated explicitly for each principal quantum number n up to $n = 25$, and then logarithmically up to $n = 999$.
- Angular momenta number ℓ are included so as to numerically converge the DR rate coefficients to <1% over the ADAS temperature range $z^2(10 - 10^7)$K.

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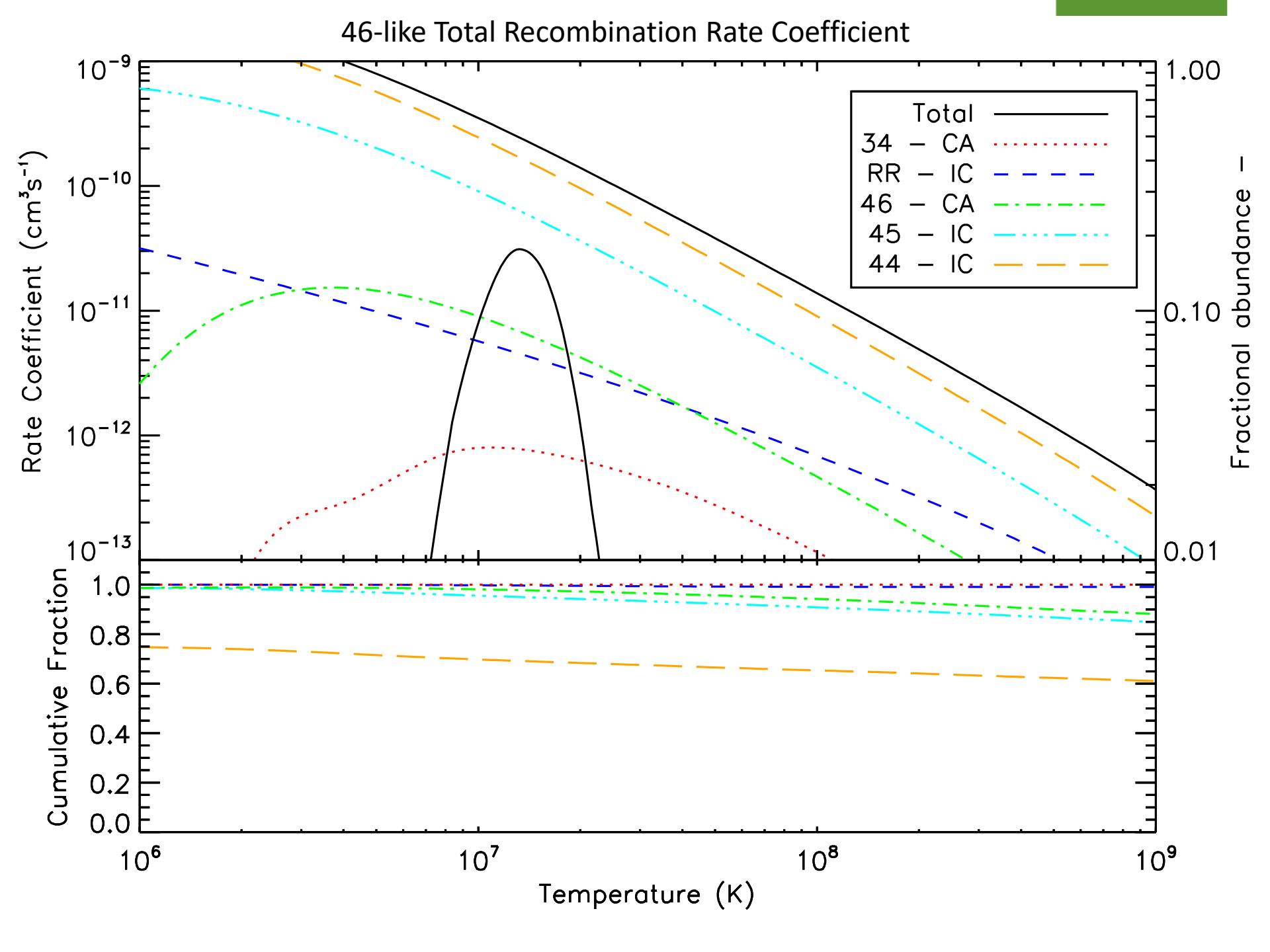
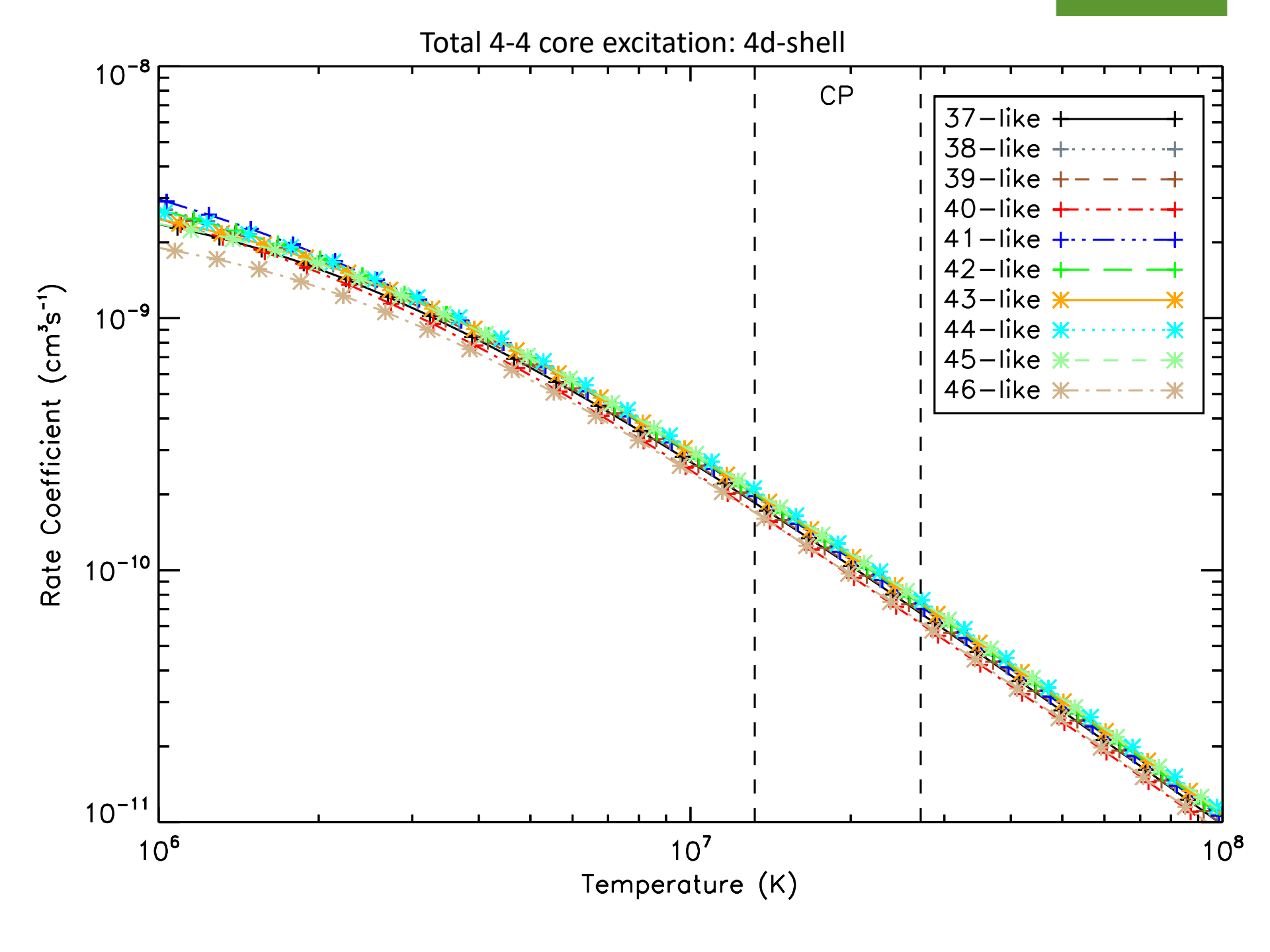
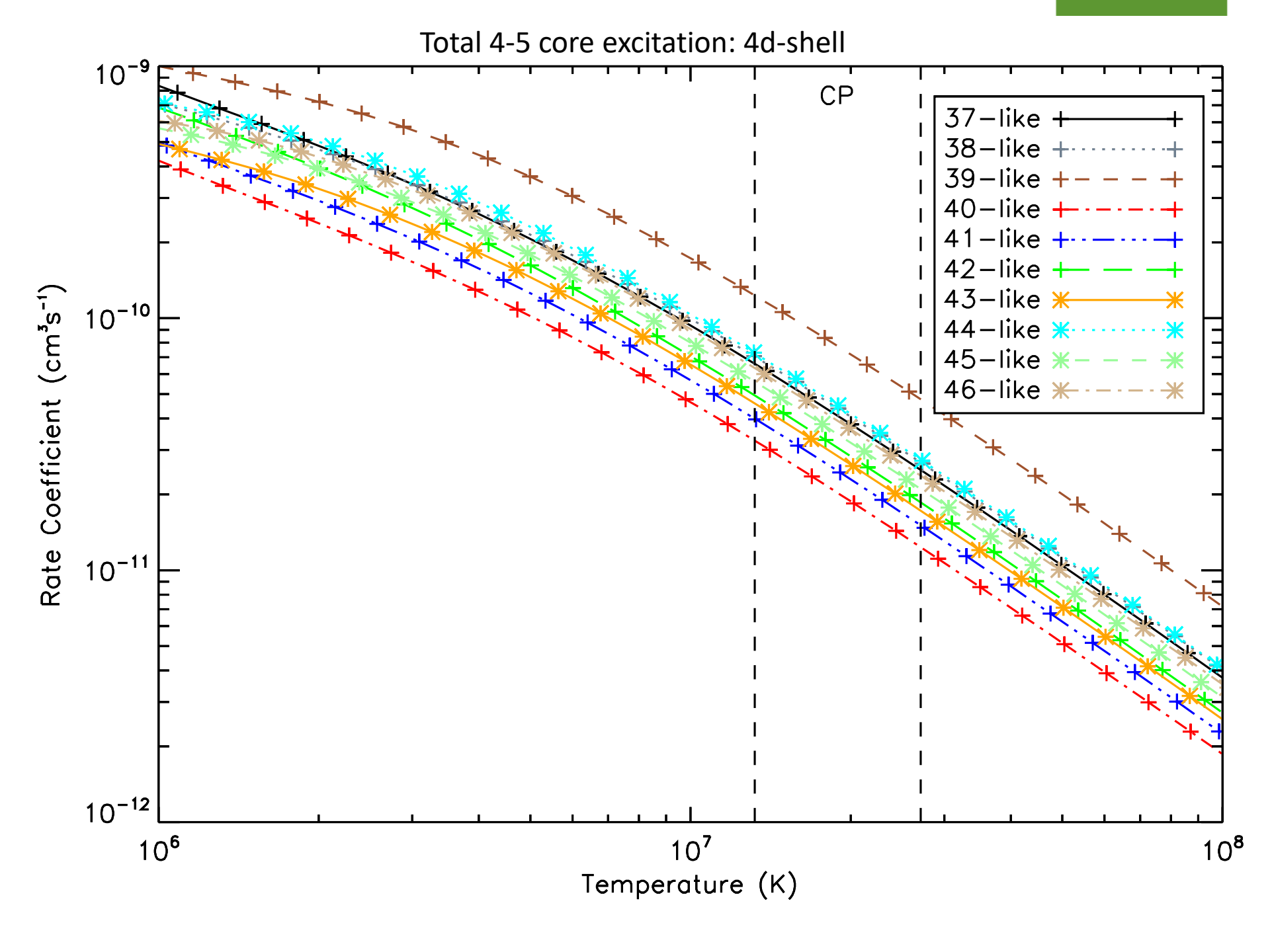
- N-electron configurations include all possible single excitations plus mixing.
- N+1-electron configurations are just N-electron with an extra electron added.
- Mixing configurations are included using the “one up-one down” rule.
- E.g. $3p^2 \rightarrow 3s\ 3d, 4p\ 4d \rightarrow 4s\ 4f$


46-like Total Recombination Rate Coefficient
Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Total
34 – CA
RR – IC
46 – CA
45 – IC
44 – IC
Cumulative Fraction
Temperature (K)


Total 4-4 core excitation: 4d-shell
CP
37−like
38−like
39−like
40−like
41−like
42−like
43−like
44−like
45−like
46−like
Rate Coefficient (cm³s⁻¹)
Temperature (K)
10⁻⁸
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁶
10⁷
10⁸


Total 4-5 core excitation: 4d-shell
CP
37−like
38−like
39−like
40−like
41−like
42−like
43−like
44−like
45−like
46−like
Rate Coefficient (cm³s⁻¹)
Temperature (K)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁶
10⁷
10⁸

Relativistic Mixing

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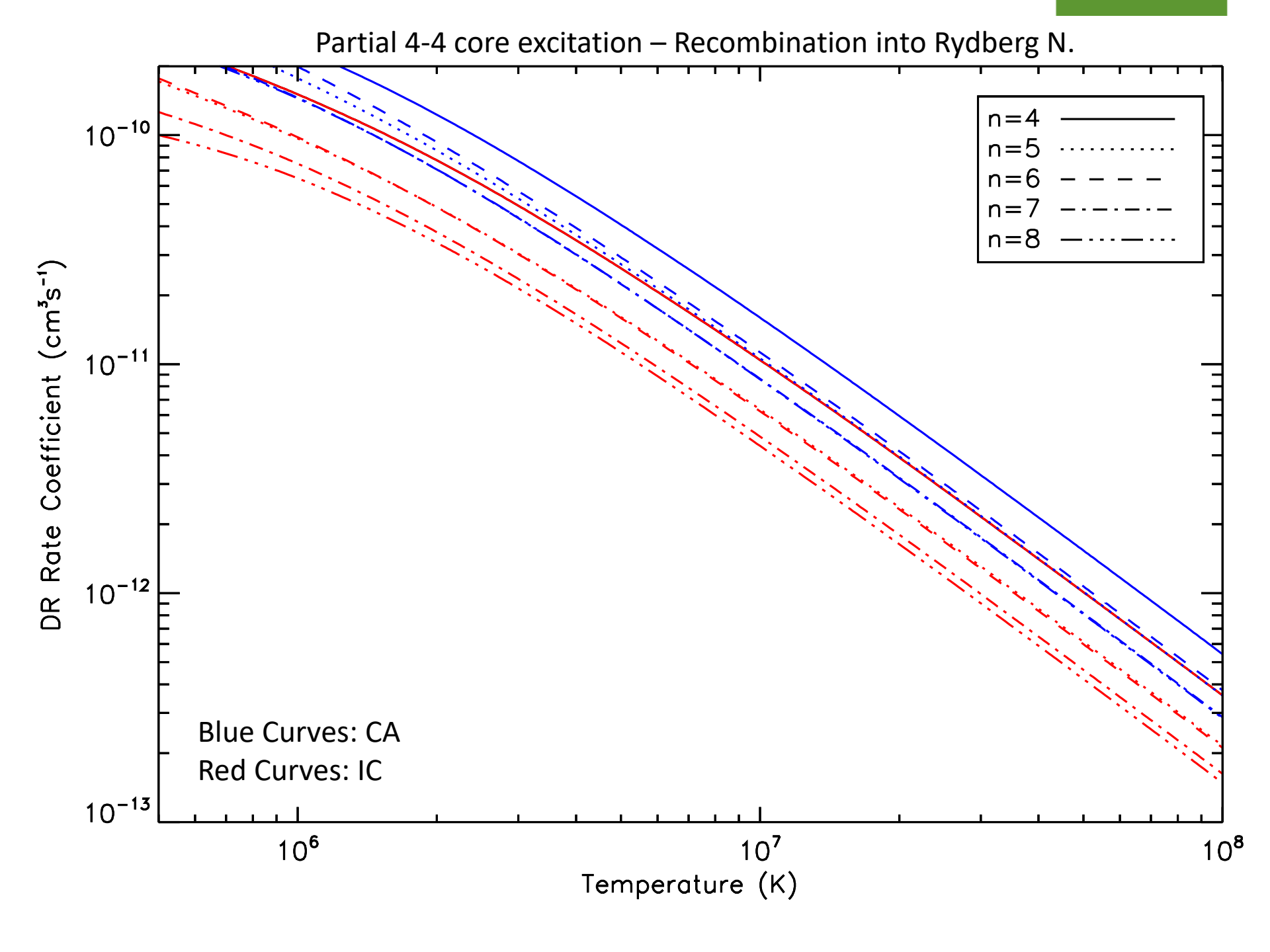
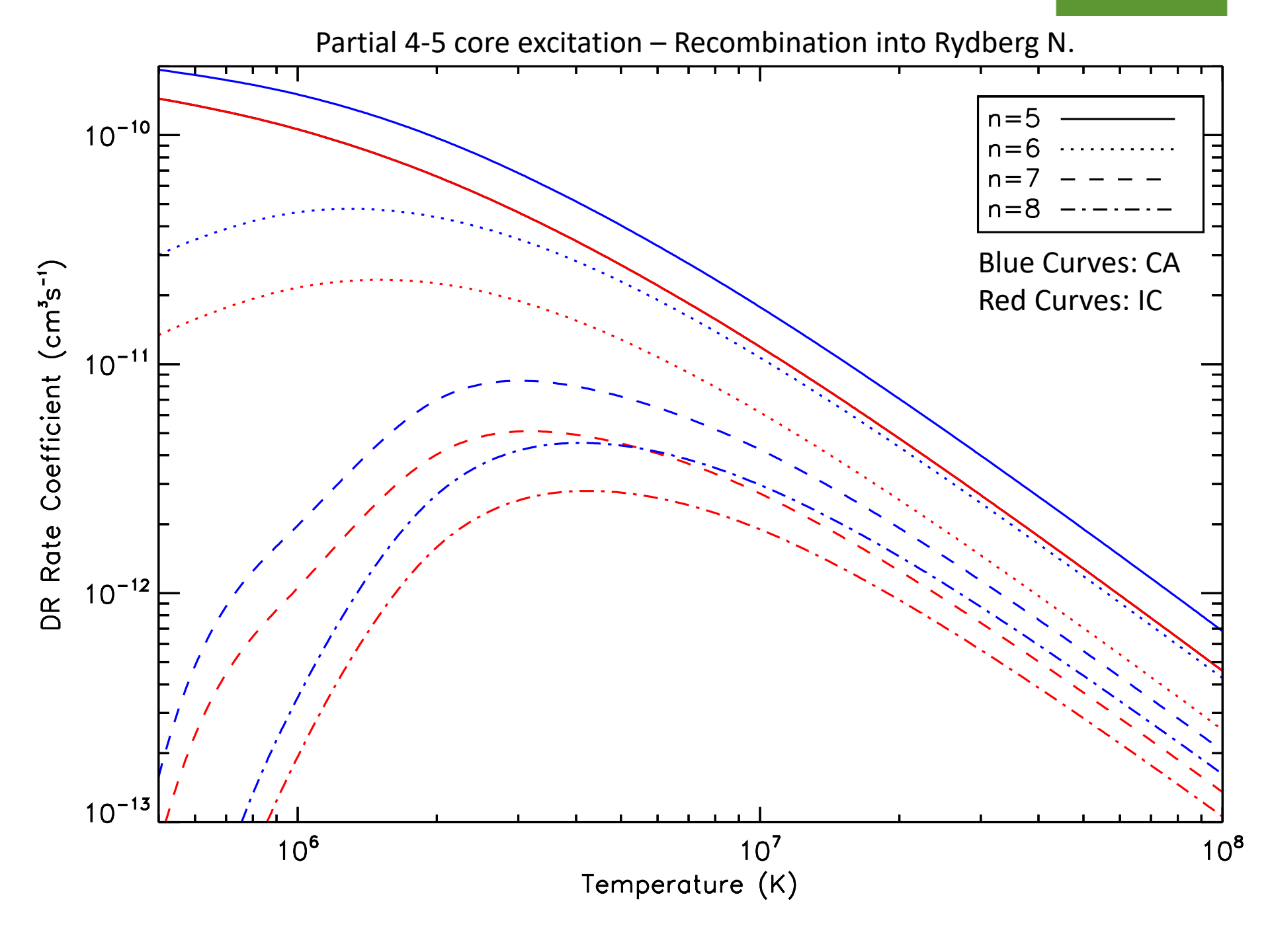
- Complete (as possible) configuration sets are required to calculate correct energies and radiative/autoionization rates.
- This has a knock-on effect on the calculated DR rate coefficient.
- Look at 30-like, core excitations 4-4 and 4-5, calculate configuration resolved (no mixing) and level resolved.


Partial 4-4 core excitation – Recombination into Rydberg N.
DR Rate Coefficient (cm³s⁻¹)
Temperature (K)
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
10⁶
10⁷
10⁸
n=4
n=5
n=6
n=7
n=8
Blue Curves: CA
Red Curves: IC


Partial 4-5 core excitation – Recombination into Rydberg N.
n=5
n=6
n=7
n=8
Blue Curves: CA
Red Curves: IC
DR Rate Coefficient (cm³s⁻¹)
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
10⁶
10⁷
10⁸
Temperature (K)

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- For 49-like onwards, splitting by core excitation no longer makes sense.
- As residual charge decreases, 5ℓ orbitals move below 4ℓ, making them energetically accessible.
- There are more accessible radiative and autoionization pathways available.

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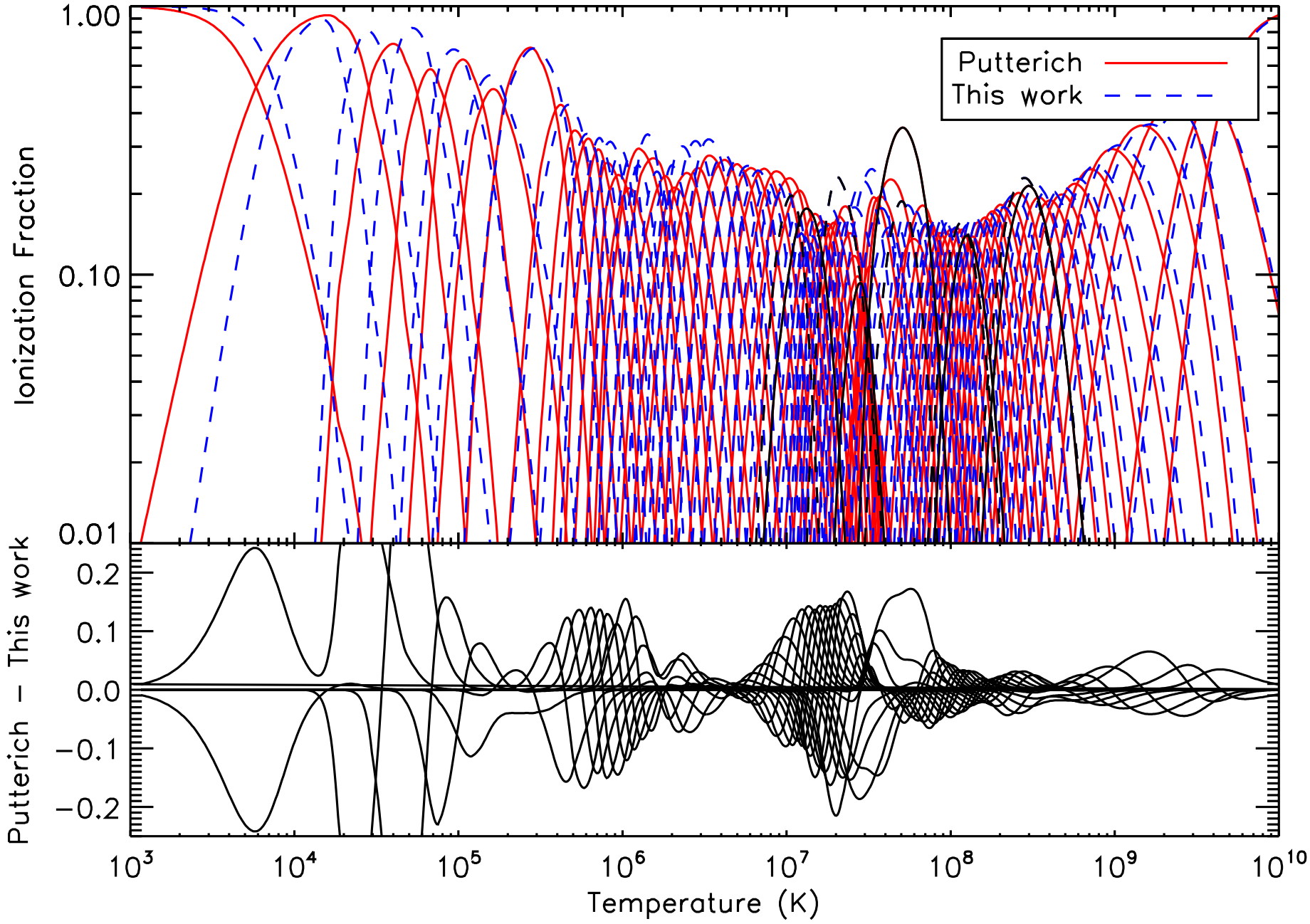
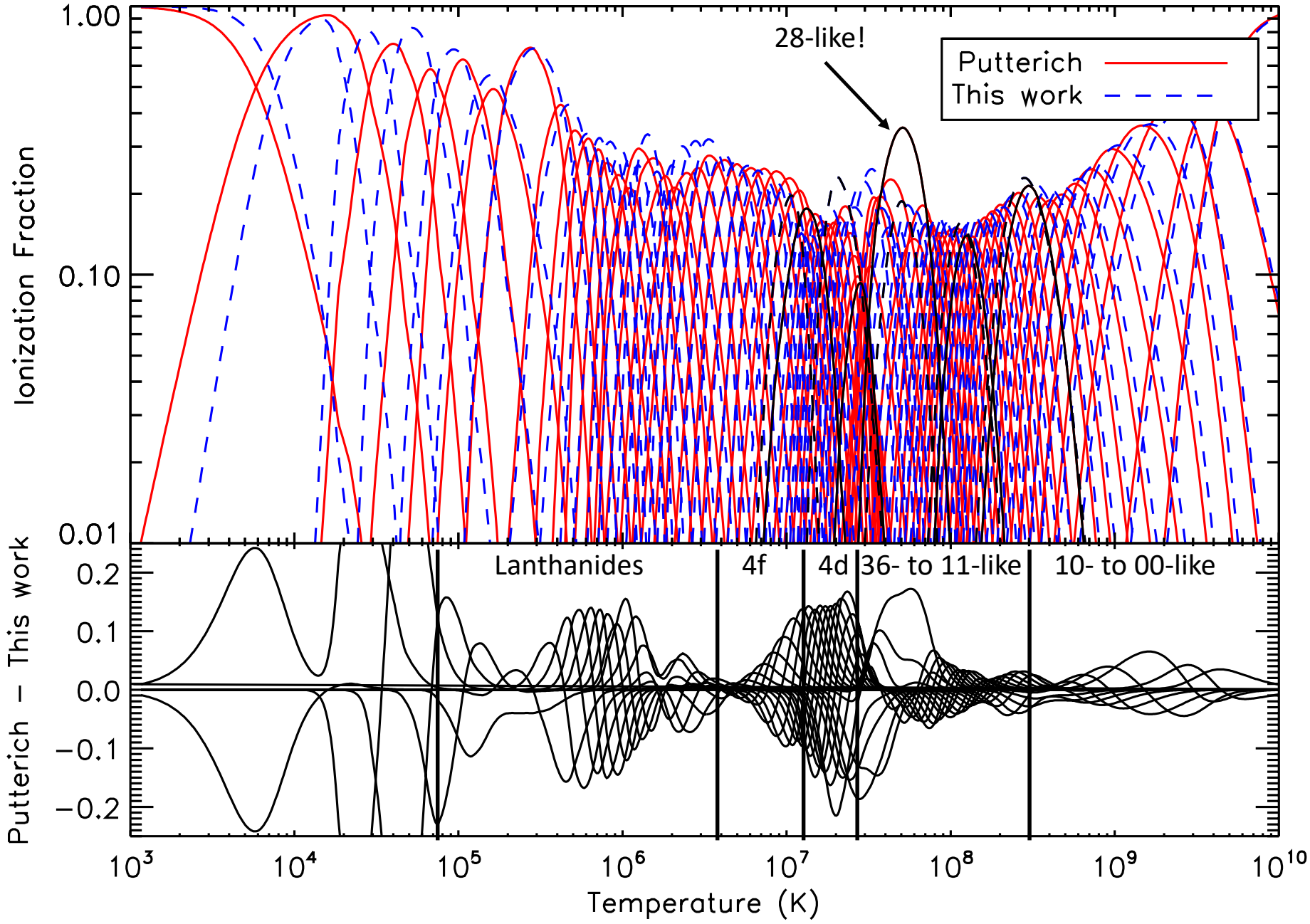
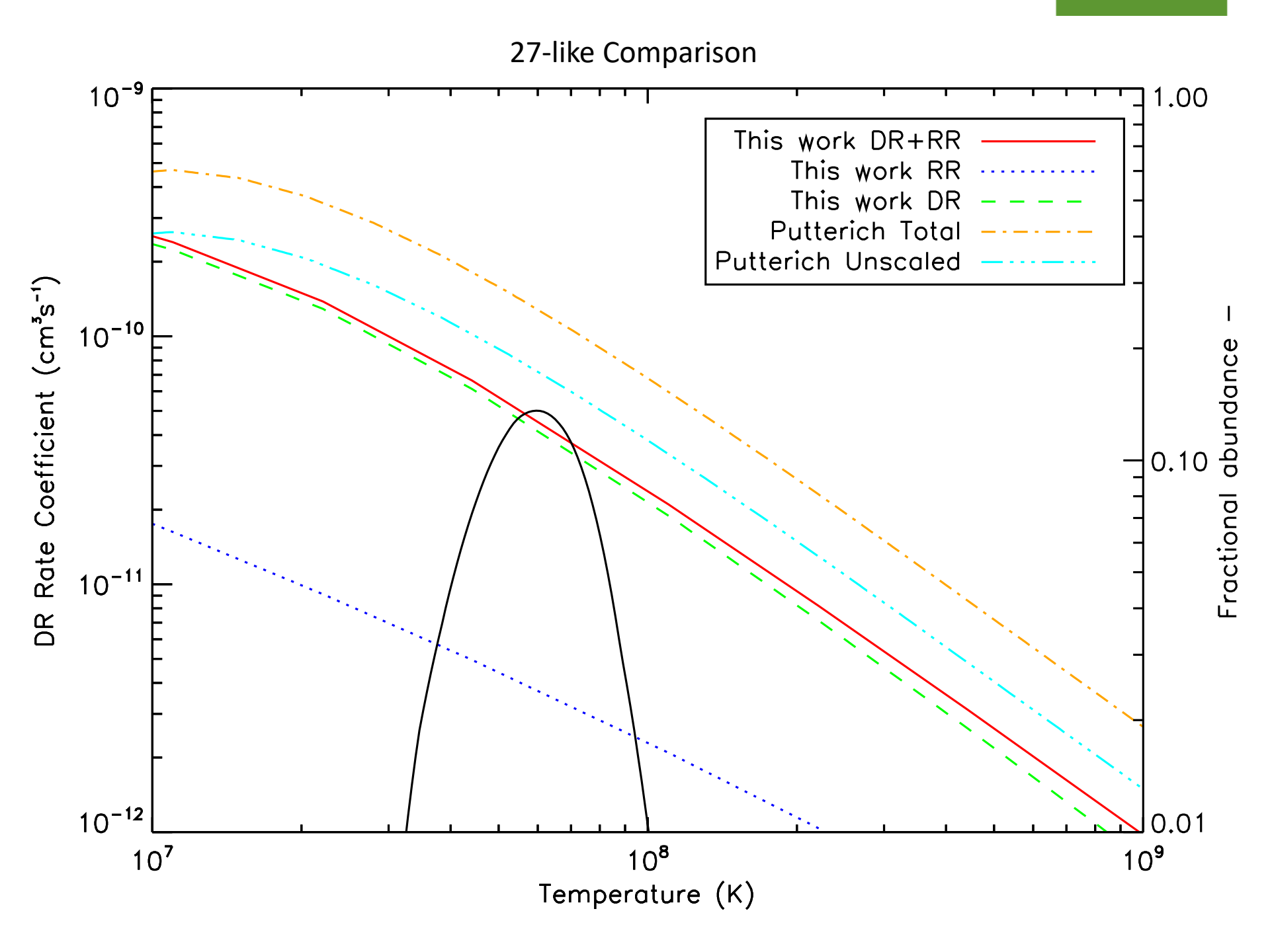
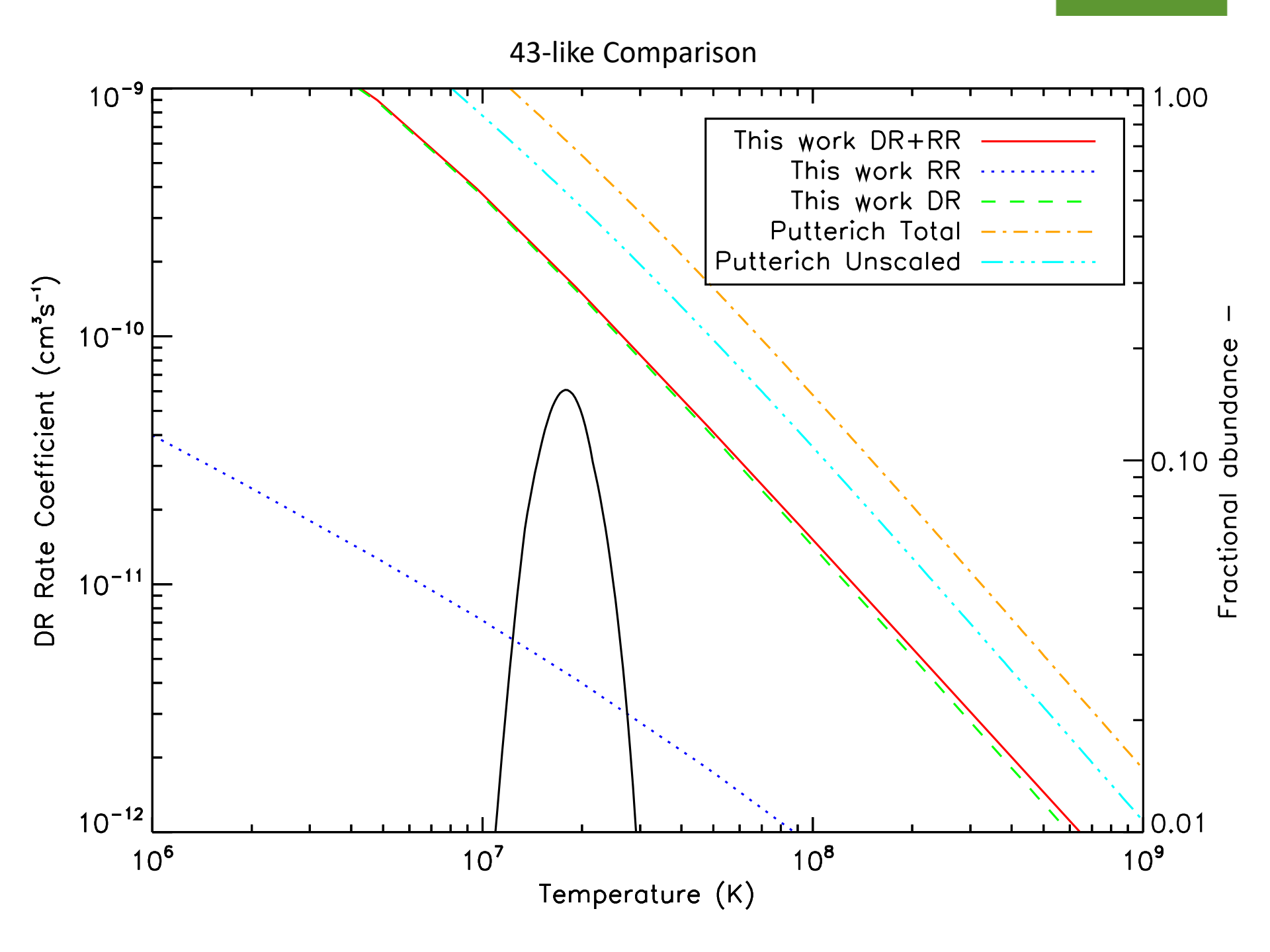
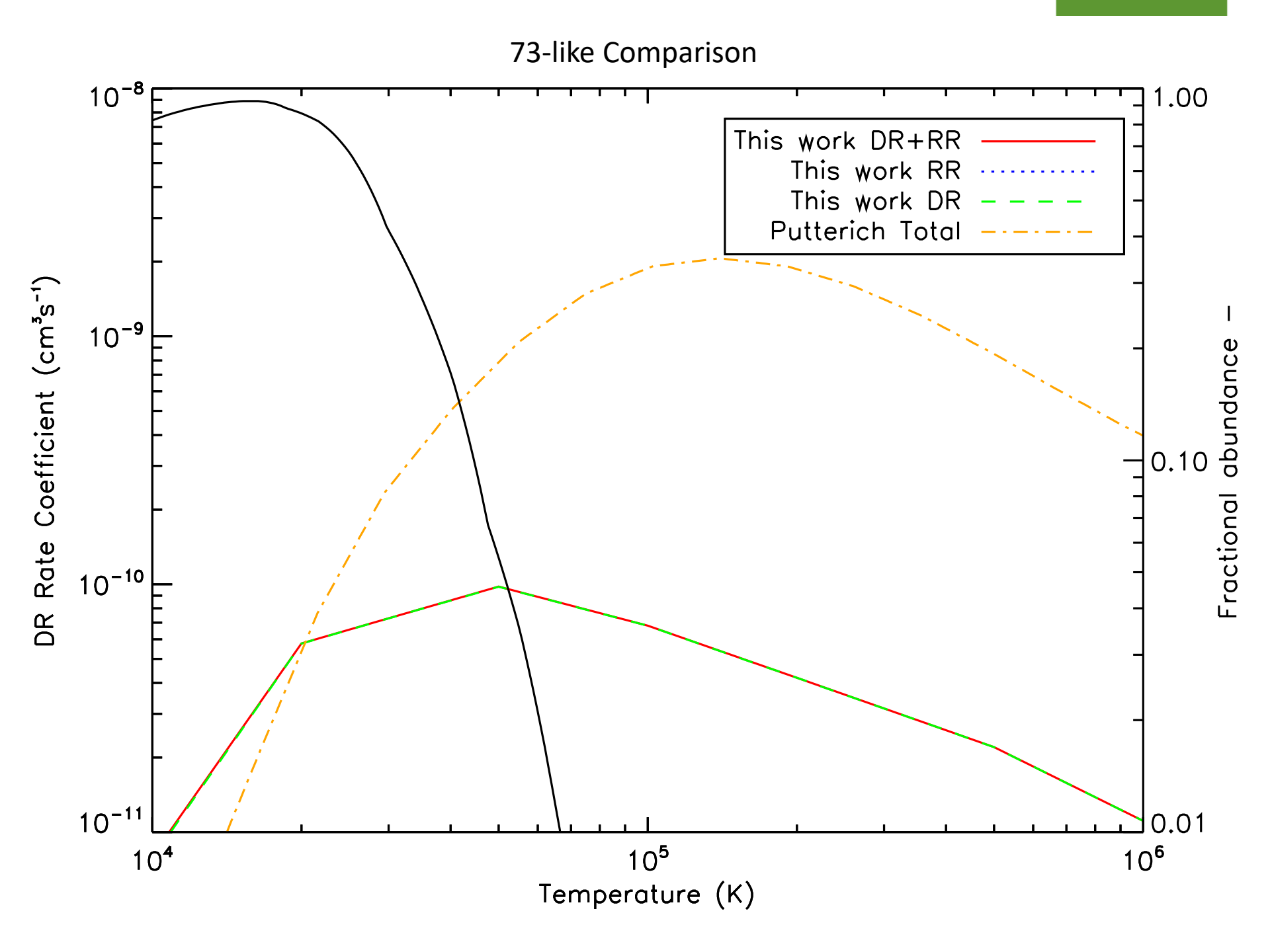
- As a first cut, calculate 49-like to 73-like in configuration average.
- For N-electron target, include all possible double promotions from ground configuration for $n = 4 - 7$, and $\ell = 0 - (n - 1)$.
- For N+1 target, include all possible triple promotions from ground over same $n\ell$ range.
- Rydberg n and ℓ the same as previous case.


Putterich
This work
Ionization Fraction
1.00
0.10
0.01
Putterich − This work
0.2
0.1
0.0
−0.1
−0.2
10^3
10^4
10^5
10^6
10^7
10^8
10^9
10^{10}
Temperature (K)


1.00
0.10
0.01
Ionization Fraction
28-like!
Putterich
This work
Lanthanides
4f
4d
36- to 11-like
10- to 00-like
0.2
0.1
0.0
−0.1
−0.2
Putterich − This work
10^3
10^4
10^5
10^6
10^7
10^8
10^9
10^10
Temperature (K)


27-like Comparison
This work DR+RR
This work RR
This work DR
Putterich Total
Putterich Unscaled
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Temperature (K)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
1.00
0.10
0.01
10⁷
10⁸
10⁹


43-like Comparison
This work DR+RR
This work RR
This work DR
Putterich Total
Putterich Unscaled
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Temperature (K)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
1.00
0.10
0.01
10⁶
10⁷
10⁸
10⁹


73-like Comparison
This work DR+RR
This work RR
This work DR
Putterich Total
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Temperature (K)
10⁻⁸
10⁻⁹
10⁻¹⁰
10⁻¹¹
1.00
0.10
0.01
10⁴
10⁵
10⁶

So… where are we now?

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Partial and total dielectronic recombination rate coefficients for W^{73+} to W^{56+}

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Partial and total dielectronic recombination rate coefficients for W^{55+} to W^{38+}

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CrossMark

So… where are we now?

- Ions $W^{73+} - W^{56+}$ (01-like – 18-like): Published.
- Ions $W^{55+} - W^{38+}$ (01-like – 18-like): Published.
- Ions $W^{37+} - W^{28+}$ (37-like – 46-like): Paper being written.
- Ions $W^{27+} - W^{12+}$ (47-like – 60-like): Redistributed configuration average results.
- Ions $W^{13+} - W^{01+}$ (61-like – 73-like): Level-resolved currently calculating.

Future Work

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- Application to other ions: Elements relevant to disruption mitigation such as argon, xenon…
- Remaining IC results for 61-like to 73-like.
- Collisional-Radiative modelling of ITER-like plasmas.

Conclusions

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- DR/RR data calculated for entire sequence of tungsten in configuration resolution. Level resolution available by November 2017.
- Significant changes to peak fractions and temperatures from baseline ADAS data.
- Configuration mixing important in calculating partial DR rate coefficients.