The Tungsten Project: Dielectronic Recombination data for Collisional-Radiative Modelling in ITER – W74+ - W38+

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Outline

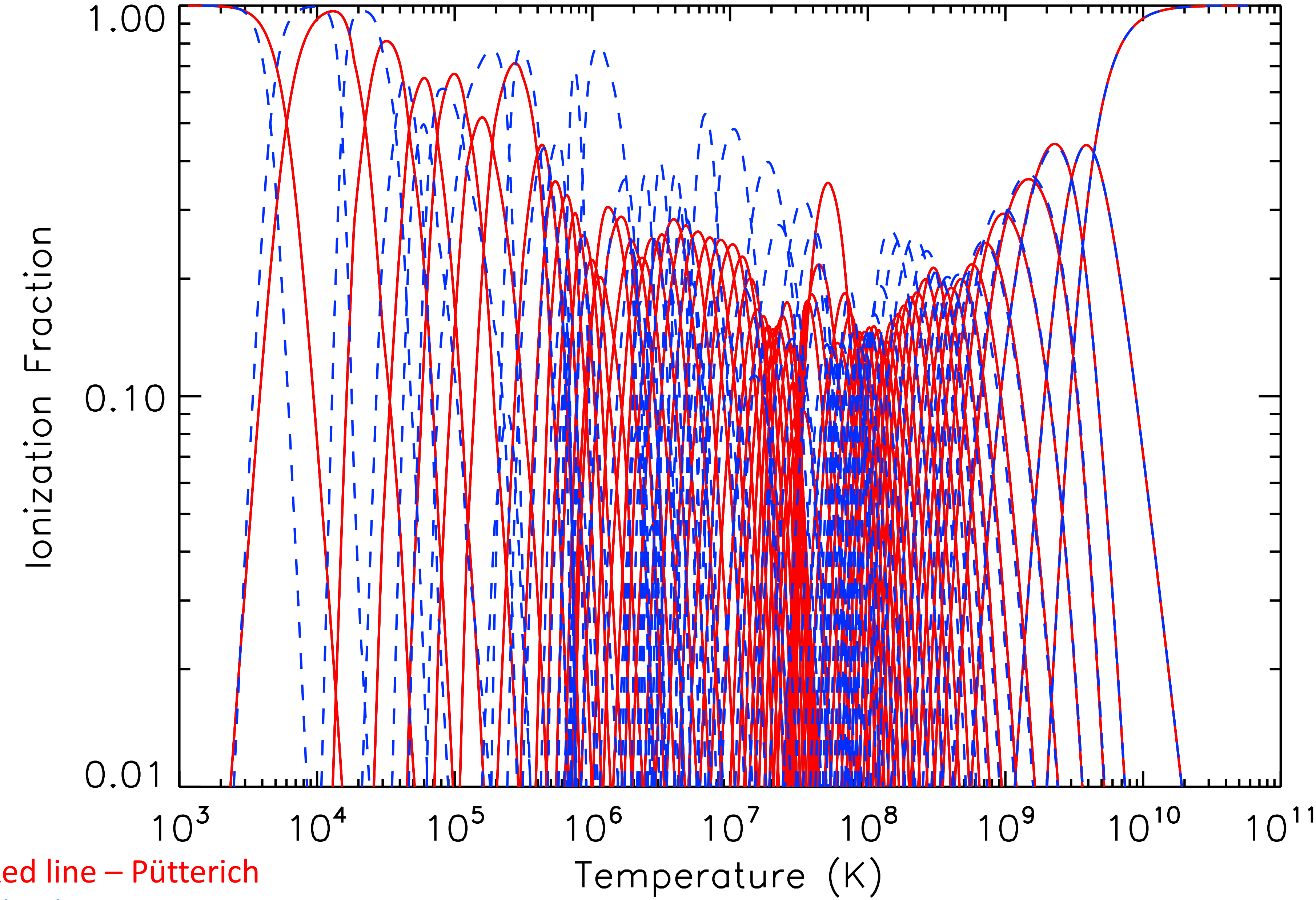
- Motivation
- The Tungsten Project
- Calculation Methods
- Results and Comparisons
- Conclusion

Motivation

- The divertor at ITER will be constructed with Tungsten.
- ITER-like wall in JET experiment shows large power losses in the plasma.
- Need to understand this from Collisional-Radiative perspective.
- Need partial final-state resolved DR/RR rate coefficients.

Motivation

- Several Tungsten DR data sets exist:
  - Pütterich et al. (2008), 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

The Tungsten Project

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- Require partial DR rate coefficients for entire isonuclear sequence of Tungsten.
- The Tungsten Project aims to be the first to calculate this data.
- Data will be hosted on OPEN-ADAS as it is published.
- Data will be calculated using AUTOSTRUCTURE (Badnell 1986, 1997, 2011)

The Tungsten Project

- 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.

The Tungsten Project

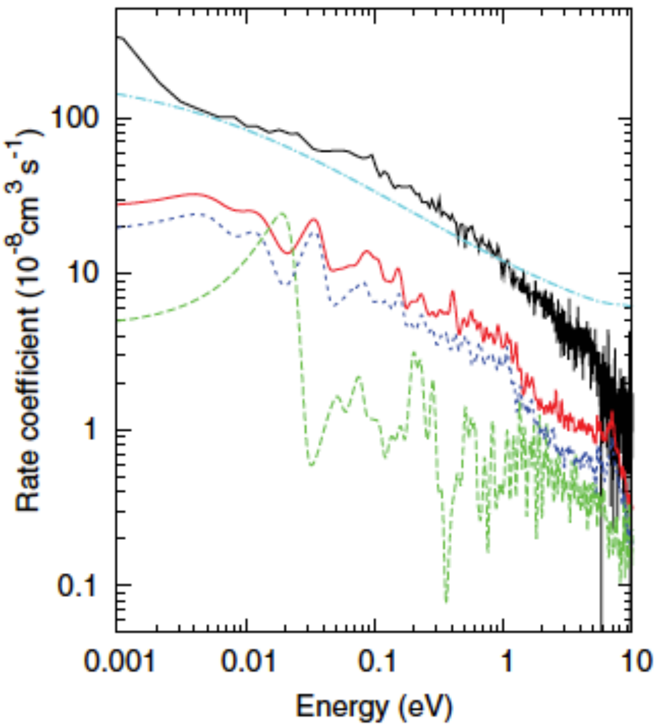


FIG. 5. (Color online) W^{20+} merged-beam DR rate coefficients: experiment [7] [upper solid (black) curve], partitioned total [dot-dashed (cyan) curve], IC total [lower solid (red) curve], *LS* total [long-dashed (green) curve], and IC $4d \rightarrow 4f$ only [short-dashed (blue) curve].

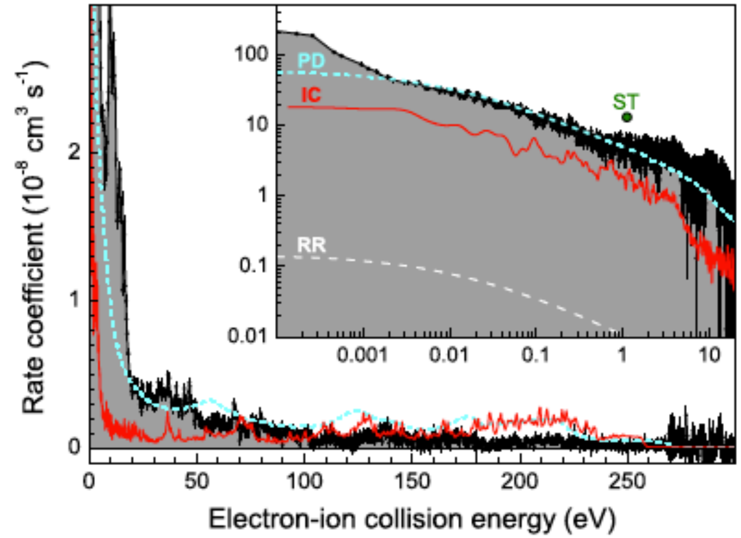


FIG. 3. (Color online) Comparison of our measured (symbols) and various calculated merged-beam recombination rate coefficients. The solid curve (labeled IC) is the result of the present intermediate-coupling calculation. The short-dashed curve (labeled PD) is the result of the fully partitioned calculation including autoionizing (and radiative) damping. The long-dashed curve (labeled RR) is the calculated rate coefficient for radiative recombination. Inset: The same data up to 20 eV on a double logarithmic scale. The full circle (labeled ST) is the rate coefficient from the statistical theory by Dzuba *et al.* [13].

Badnell (2011) – W20+

Spruck (2014) – W18+

The Tungsten Project

- 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.

The Tungsten Project

- 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 it's contribution to the total in configuration average.

The Tungsten Project

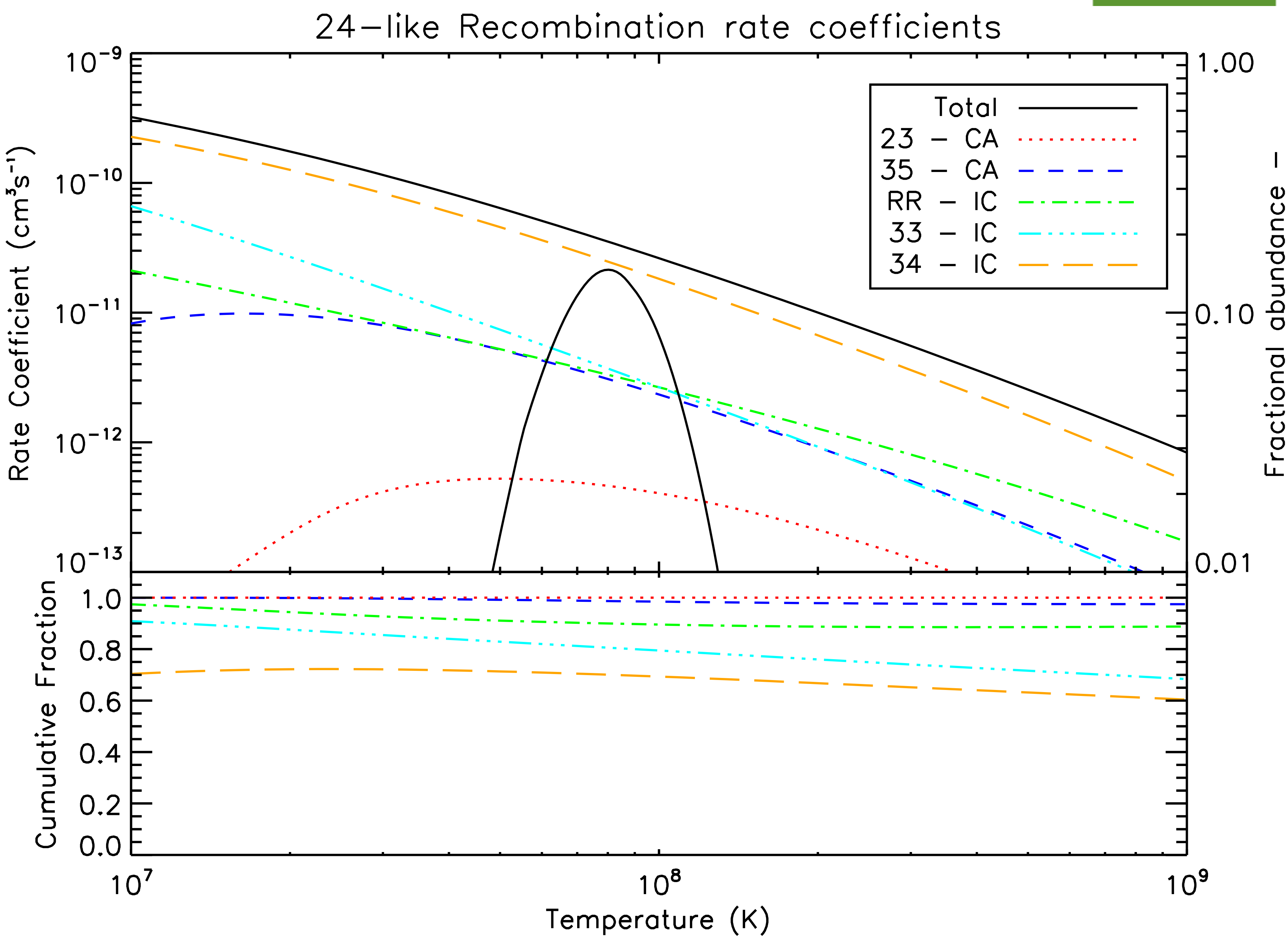
- Summing over autoionizing states, the Rydberg electron is calculated explicitly for each principal quantum number n up to $n = 25$, and then logarithmically up to $n = 999$.
- Angular momenta number ℓ are included so as to numerically converge the DR rate coefficients to <1% over the ADAS temperature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

The Tungsten Project

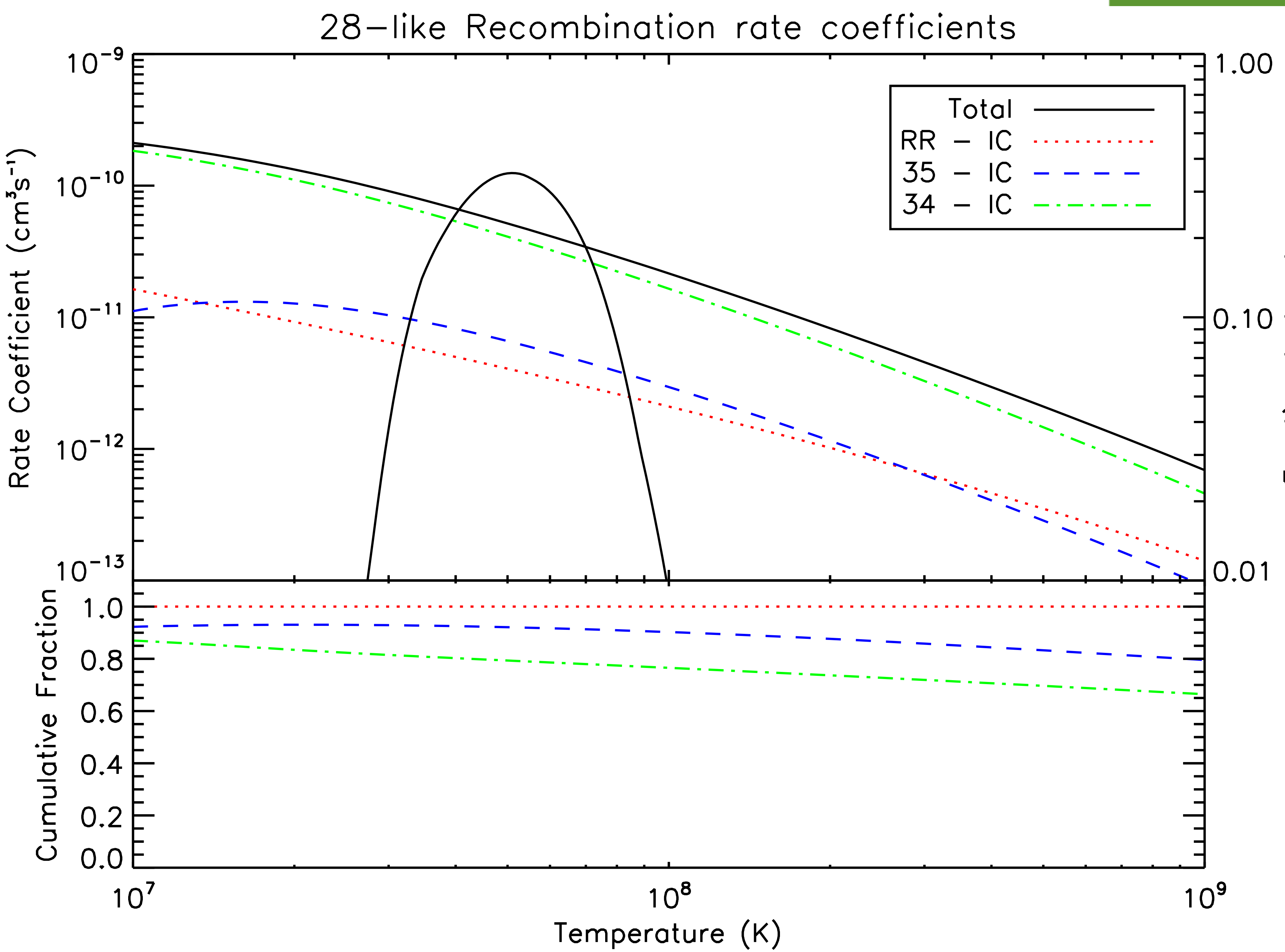
- N-electron configurations include all possible single excitations plus mixing.
- N+1-electron configurations are just N-electron with an extra electron added.
- Mixing configurations are included using the "one up-one down" rule.
- E.g. $3p^2 \rightarrow 3s\ 3d,\ 4p\ 4d \rightarrow 4s\ 4f$

Example: 16-like 3-3 Configs

N-electron target	N+1-electron target
$3s^2 3p^4$	$3s^2 3p^5$
$3s^2 3p^3 3d$	$3s^2 3p^4 3d$
$3s 3p^5$	$3s^2 3p^3 3d^2$
$3s 3p^4 3d$	$3s 3p^6$
$* \, 3p^6$	$3s 3p^5 3d$
$* \, 3s^2 3p^2 3d^2$	$3s 3p^4 3d^2$
	$3p^6 3d$
	$3s^2 3p^2 3d^3$

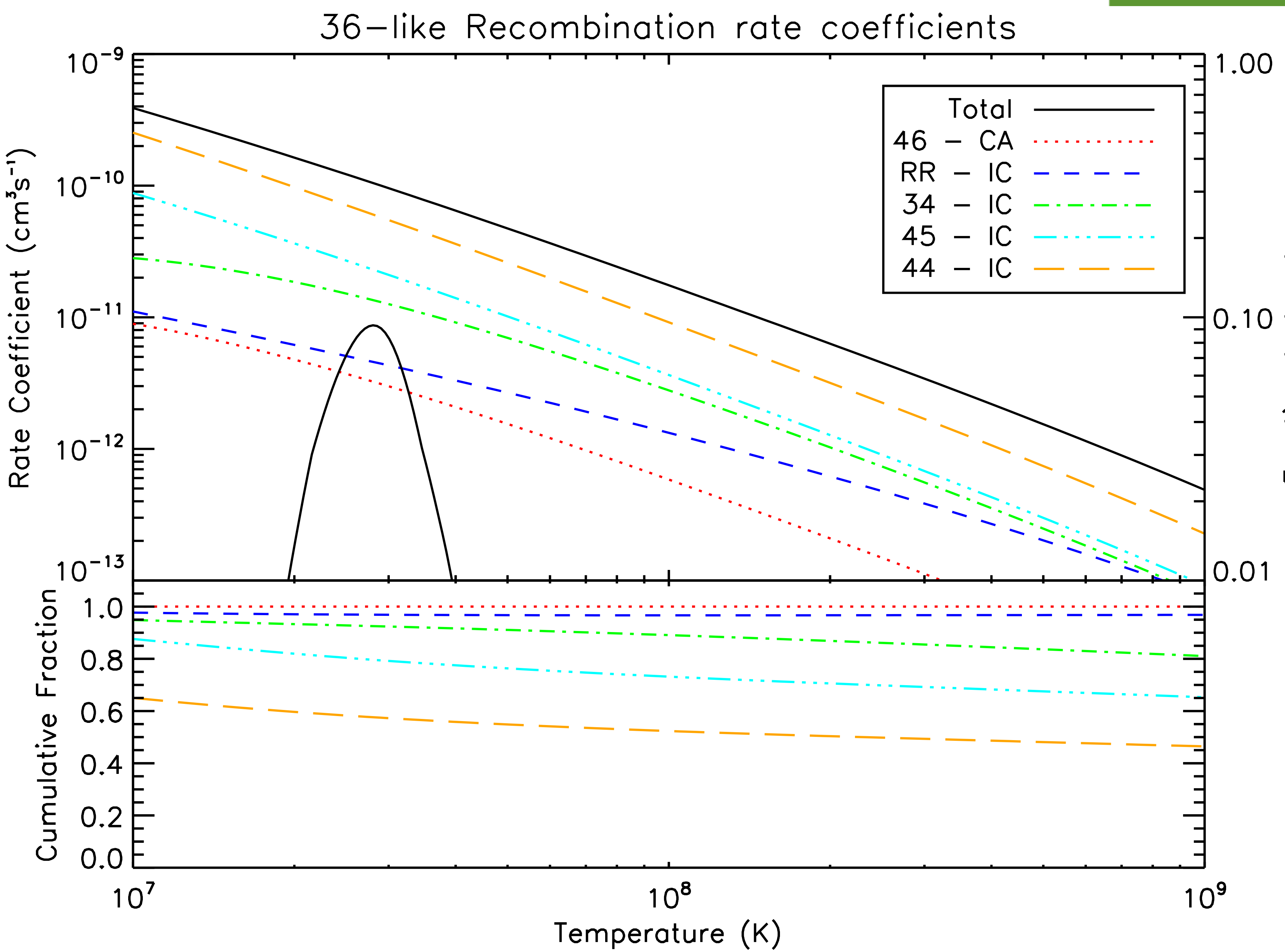

24−like Recombination rate coefficients
Total
23 − CA
35 − CA
RR − IC
33 − IC
34 − IC
Rate Coefficient (cm³s⁻¹)
Fractional abundance −
Cumulative Fraction
Temperature (K)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
1.00
0.10
0.01
1.0
0.8
0.6
0.4
0.2
0.0
10⁷
10⁸
10⁹

JET 2016

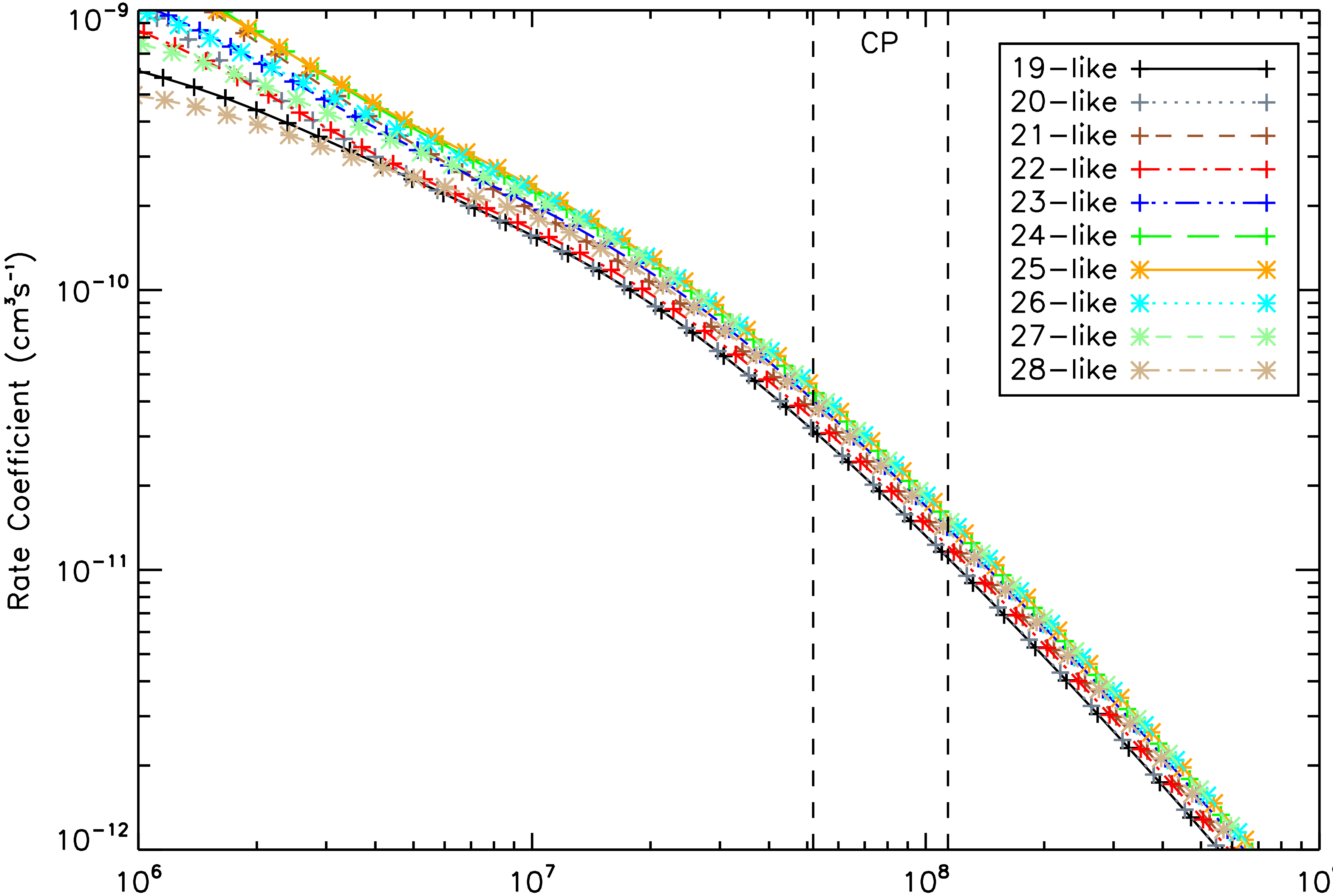


28-like Recombination rate coefficients
Total
RR – IC
35 – IC
34 – IC
Rate Coefficient (cm³s⁻¹)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
Fractional abundance –
1.00
0.10
0.01
Cumulative Fraction
1.0
0.8
0.6
0.4
0.2
0.0
10⁷
10⁸
10⁹
Temperature (K)

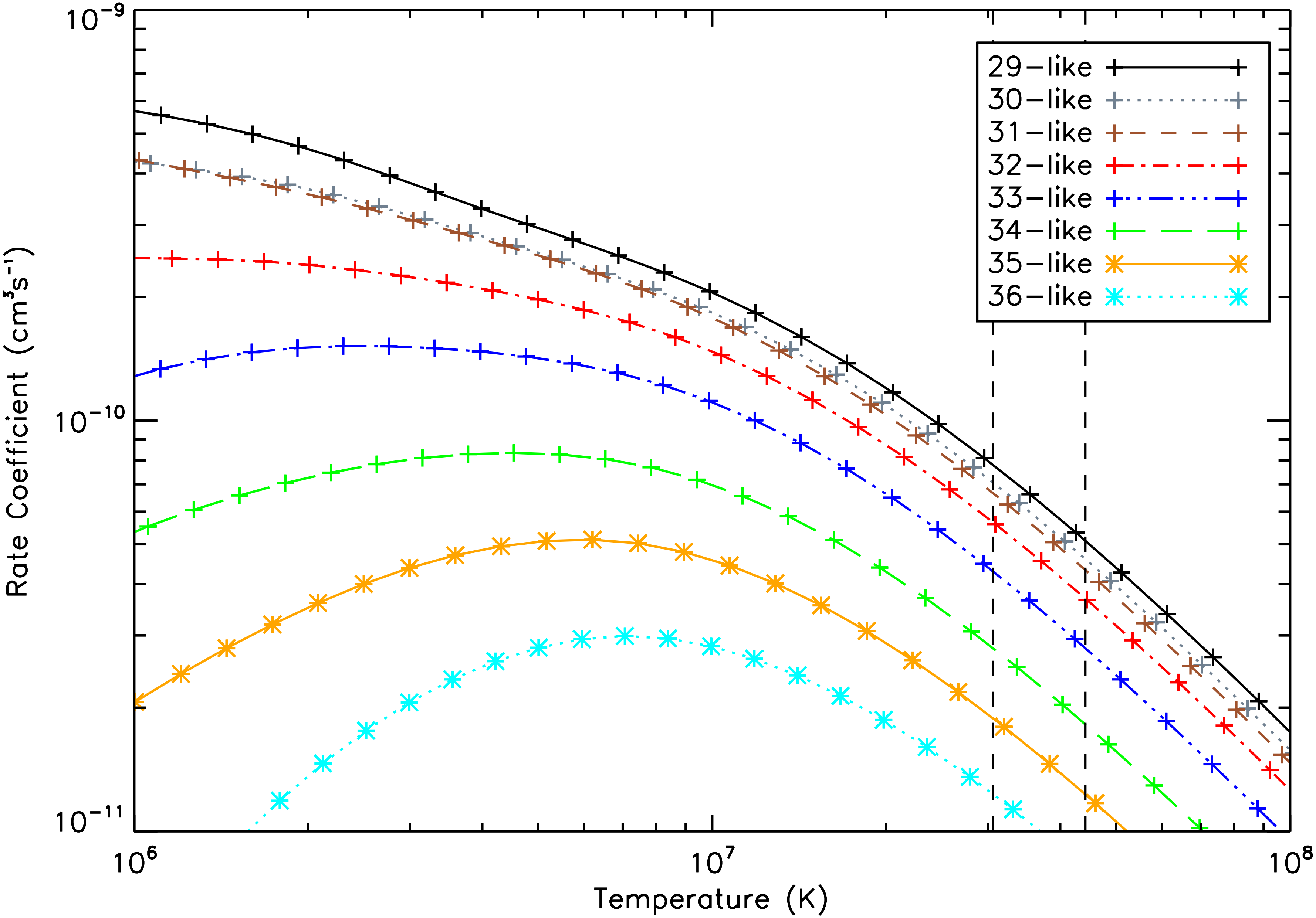
JET 2016

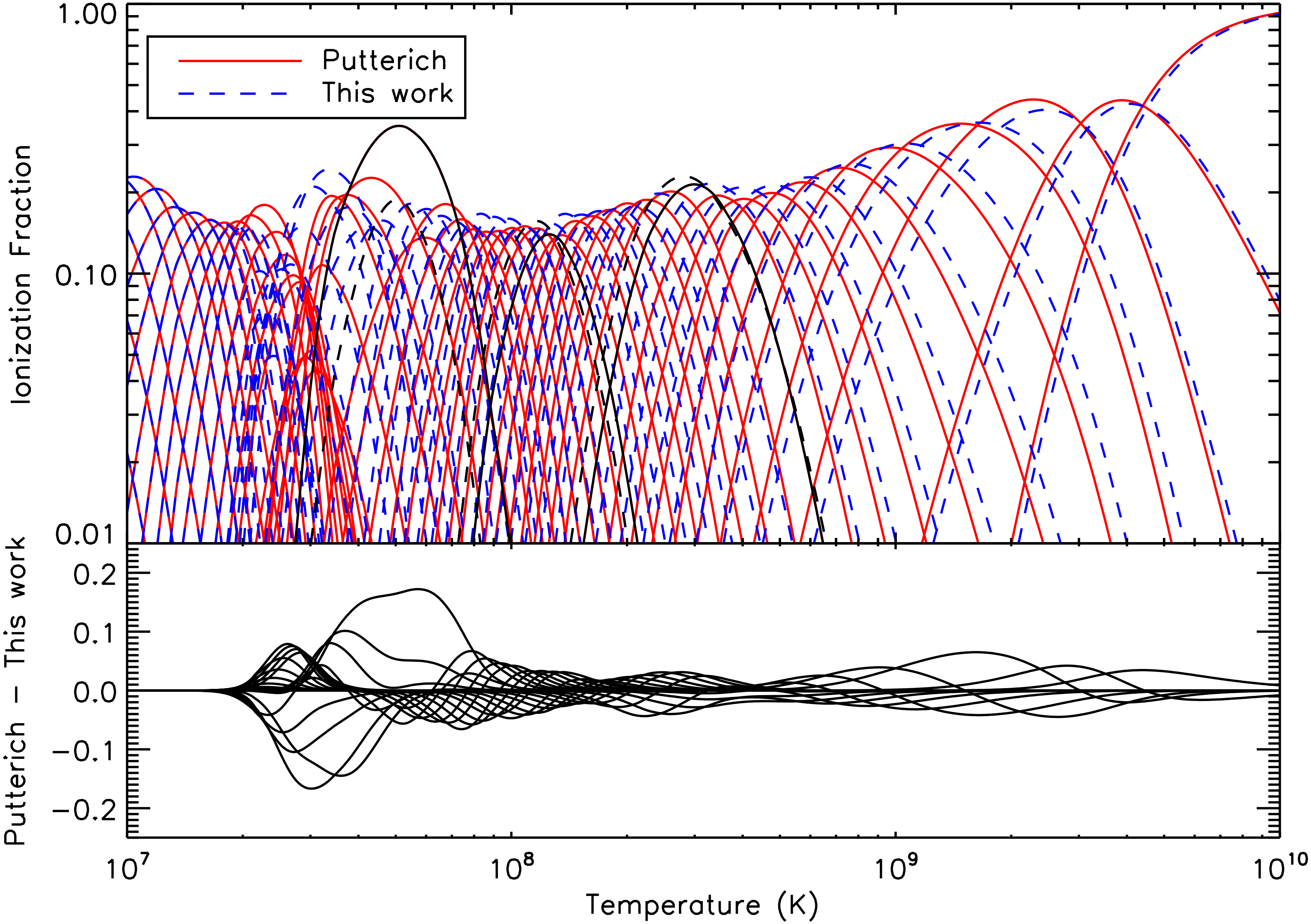

36-like Recombination rate coefficients
Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Cumulative Fraction
Temperature (K)
Total
46 – CA
RR – IC
34 – IC
45 – IC
44 – IC
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
1.00
0.10
0.01
1.0
0.8
0.6
0.4
0.2
0.0
10⁷
10⁸
10⁹
JET 2016

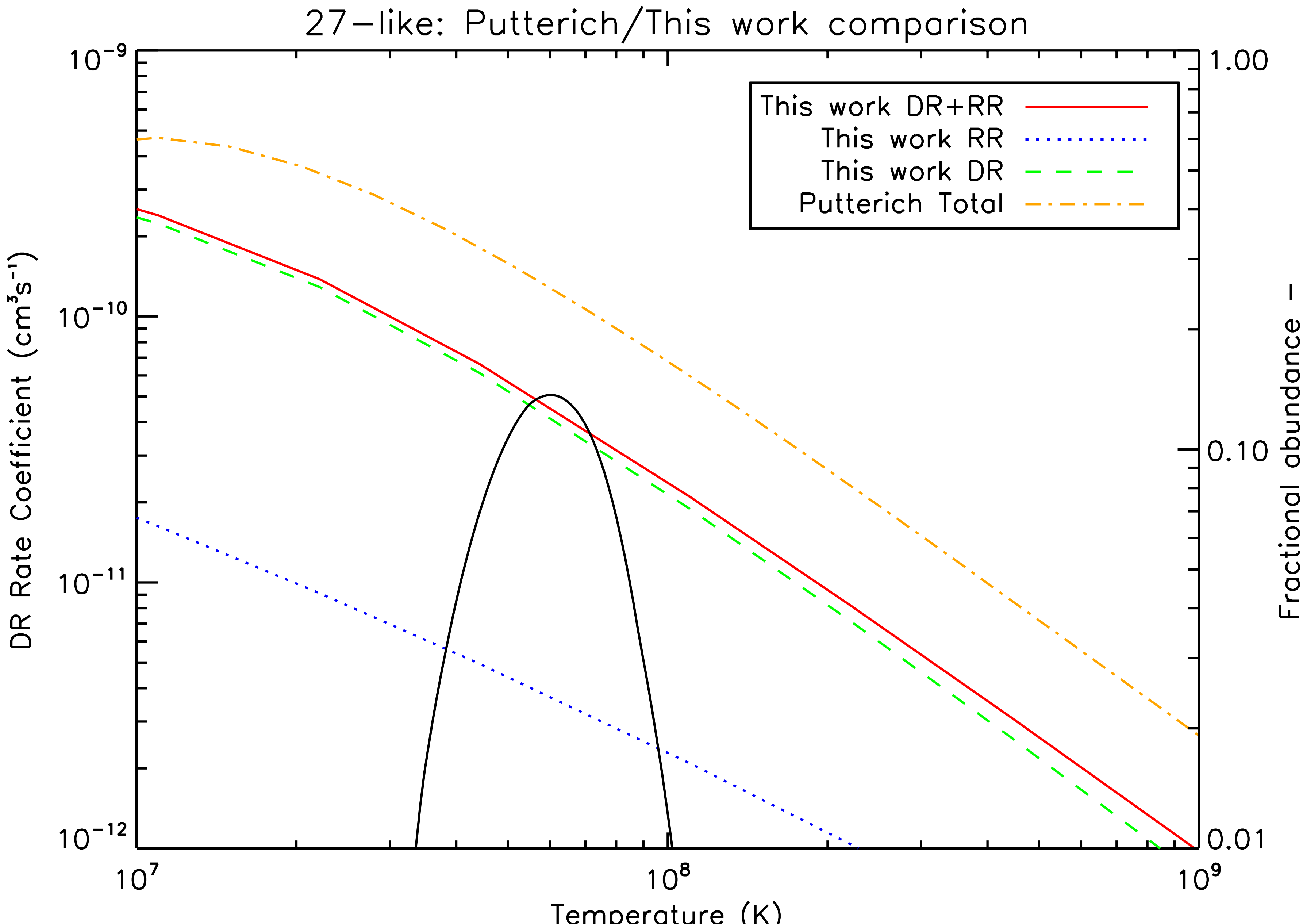
IC Total DR rate coefficients 3-4

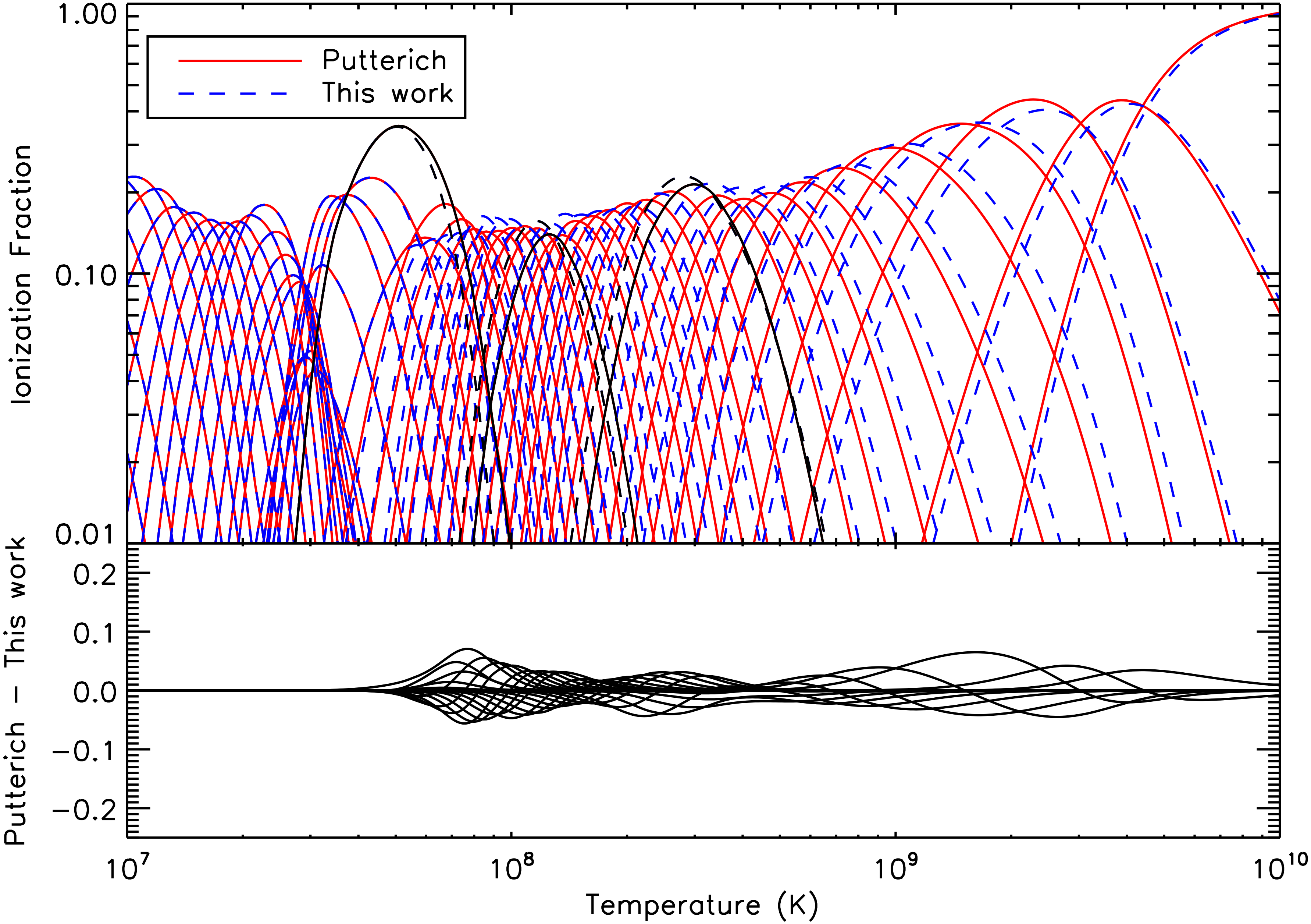


IC Total DR rate coefficients 3-4




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


27−like: Putterich/This work comparison
This work DR+RR
This work RR
This work DR
Putterich Total
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

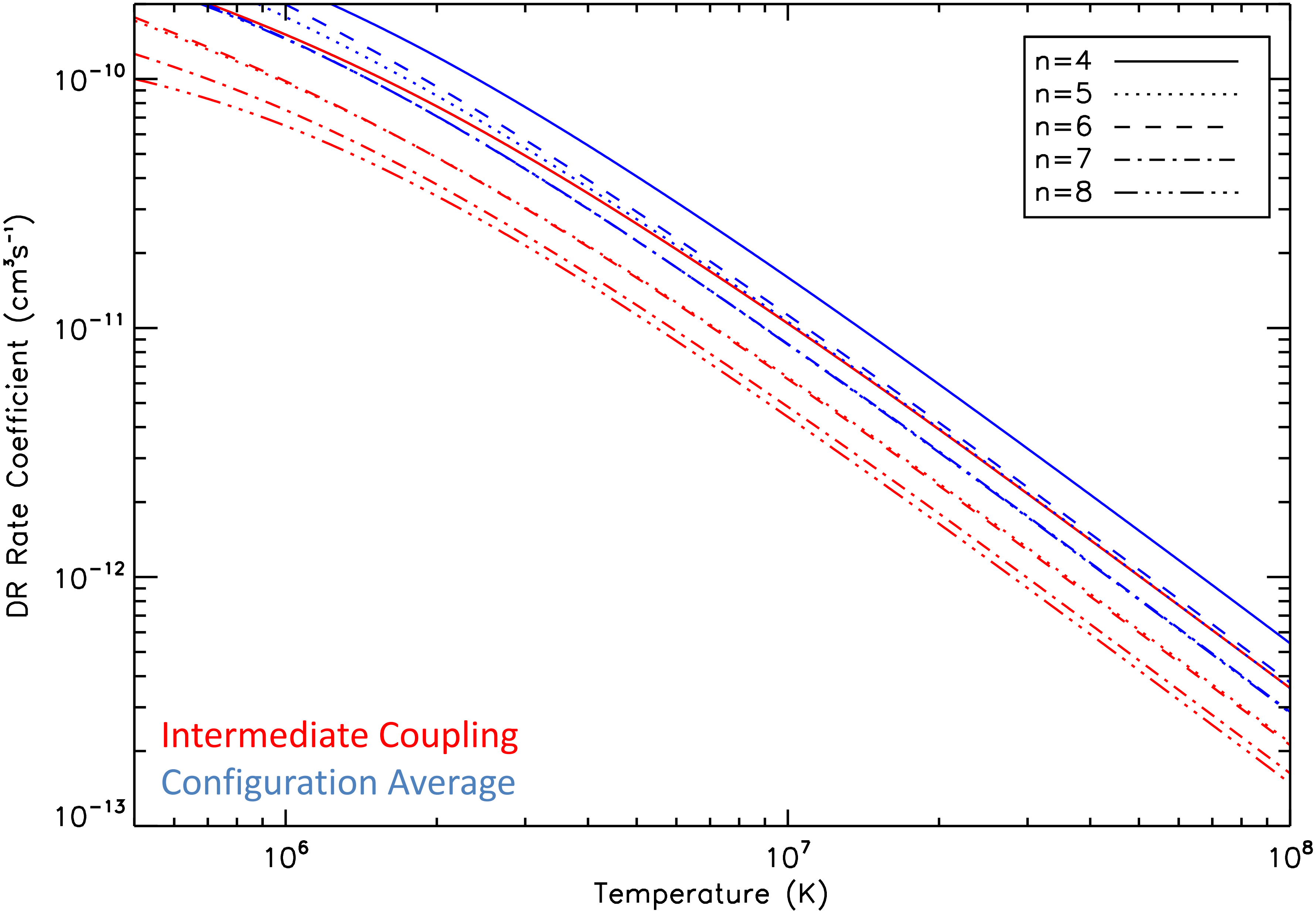


Putterich
This work
1.00
0.10
0.01
Ionization Fraction
0.2
0.1
0.0
−0.1
−0.2
Putterich − This work
10^7
10^8
10^9
10^{10}
Temperature (K)

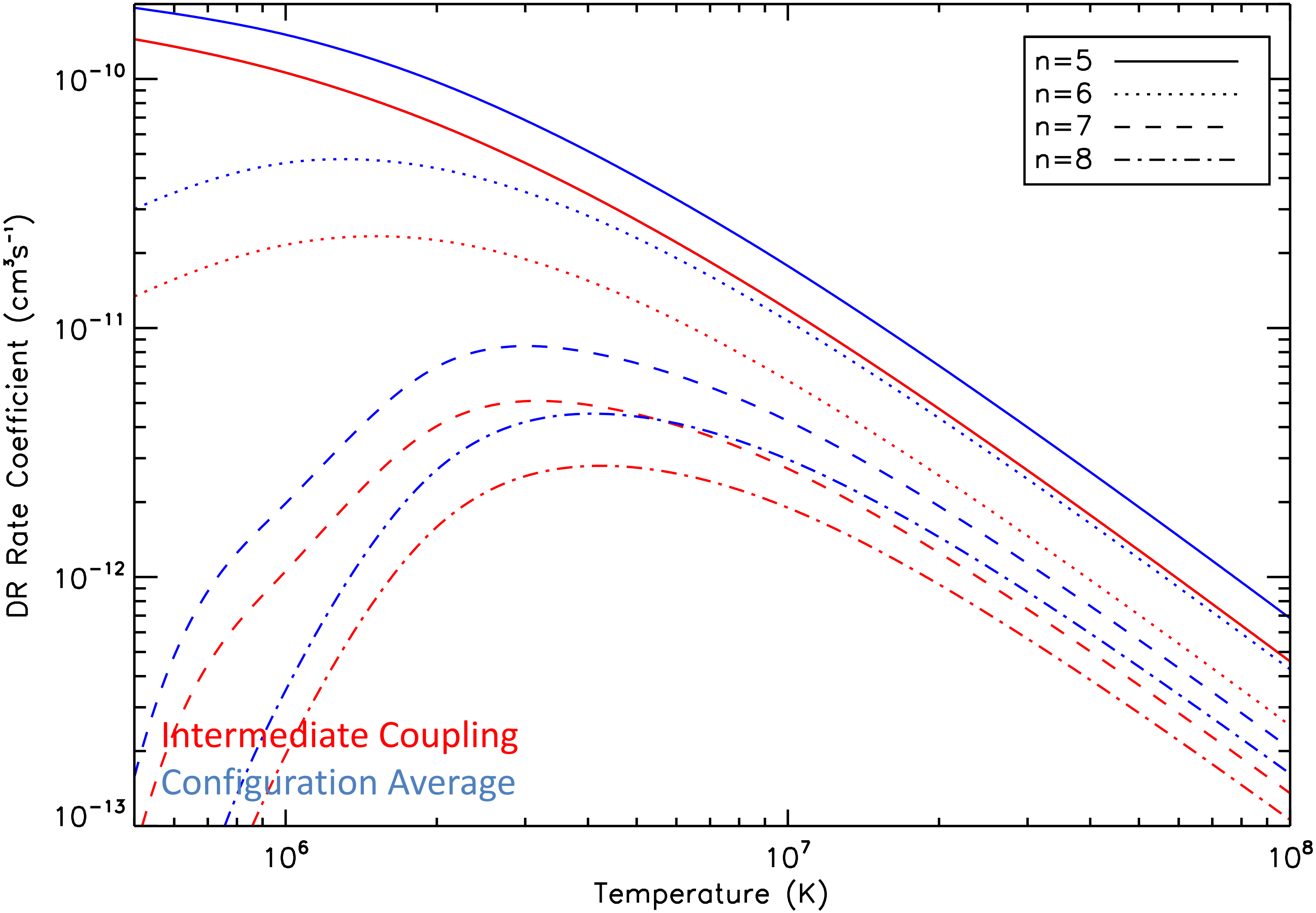
CA vs IC – Include mixing!

- CA is good for diagnostic purposes, but IC should be used when possible.
- Differences of ~80% observed between IC and CA partial DR rate coefficients.

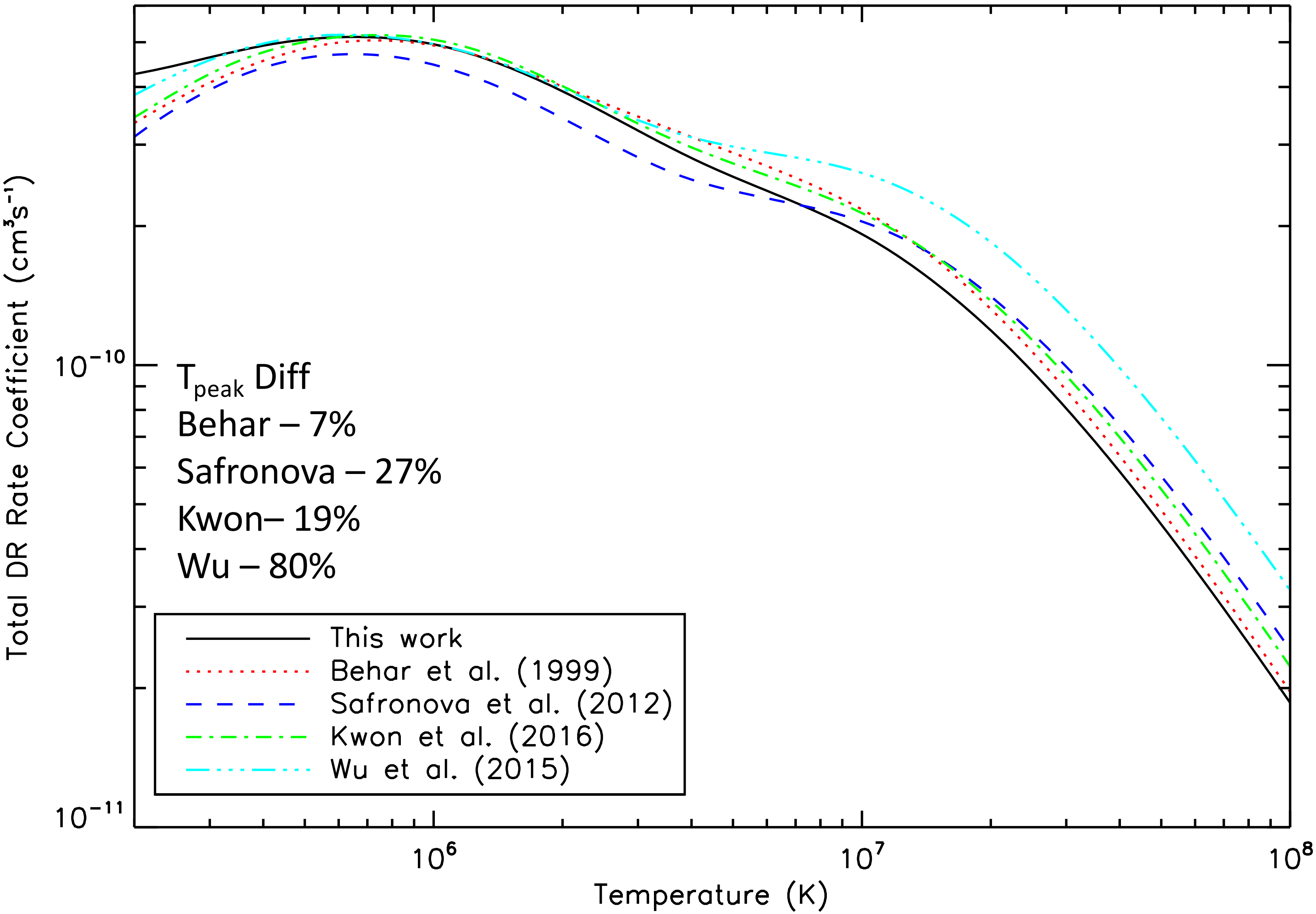
30-like Partial DR rate coefficient: 4-4



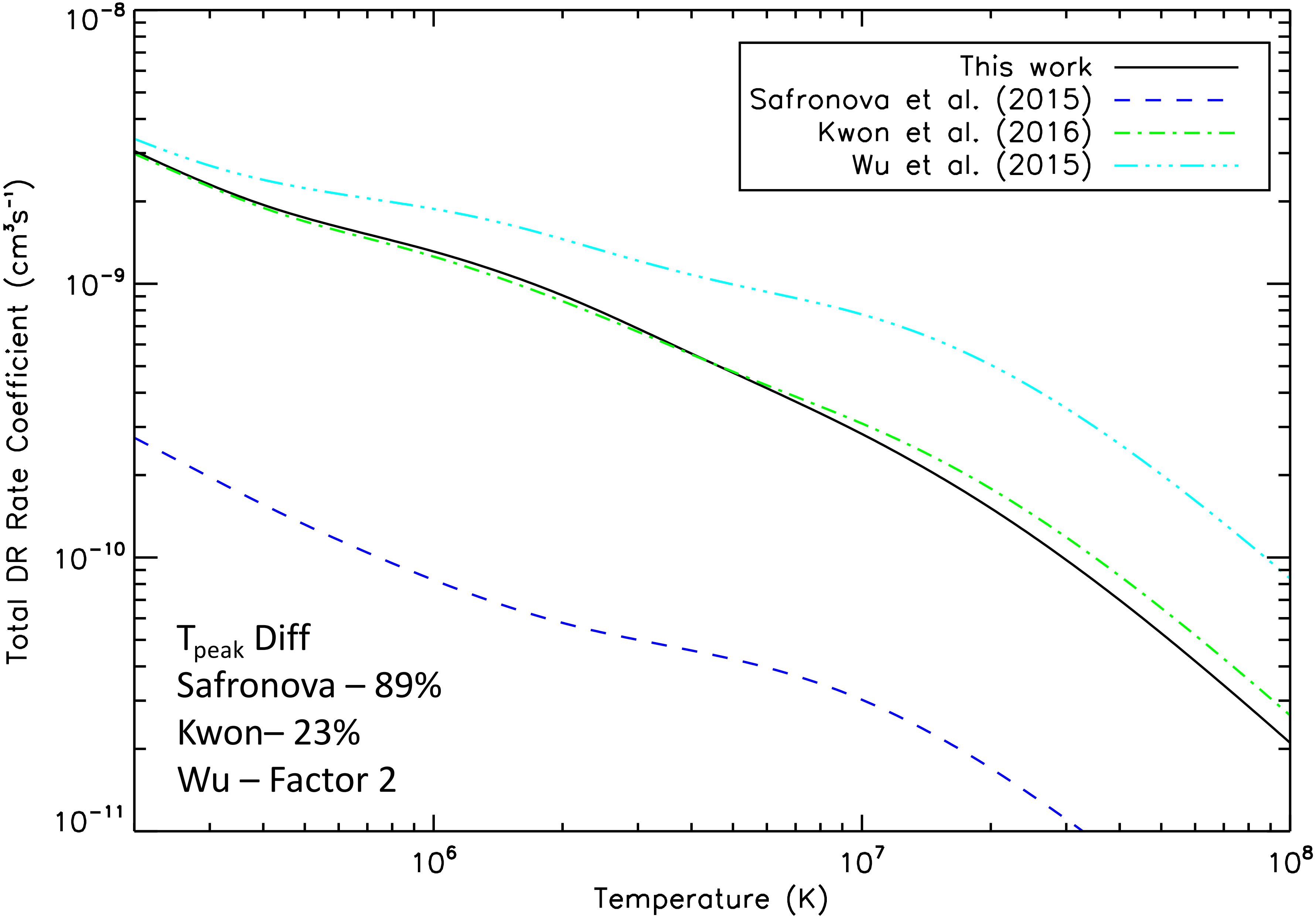
30-like Partial DR rate coefficient: 4-5



W46+ Comparison



W45+ Comparison



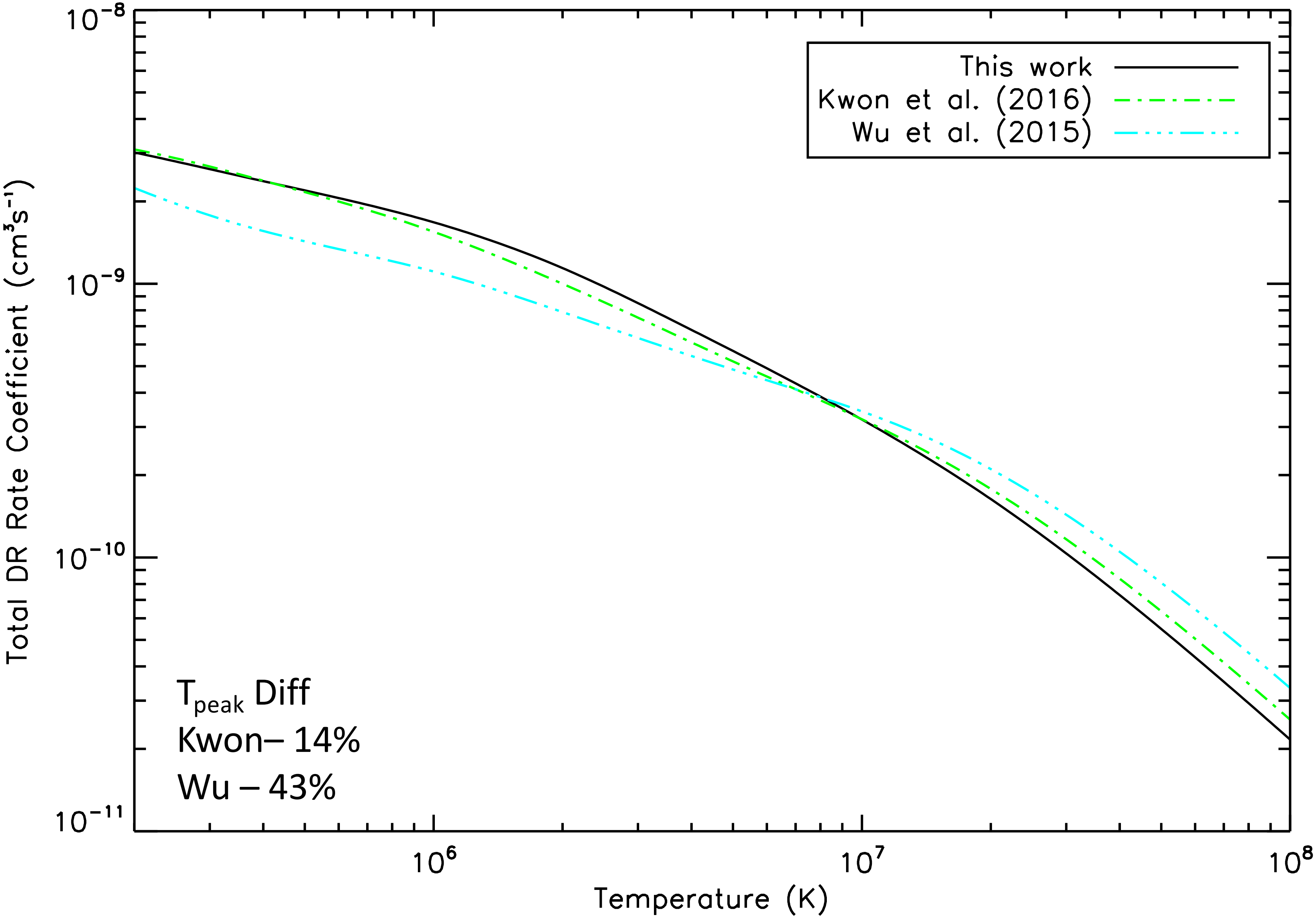
T_{peak} Diff

Safronova – 89%

Kwon– 23%

Wu – Factor 2

W44+ Comparison



So… where are we now?

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PHYSICAL REVIEW A **93**, 042703 (2016)

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

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Dielectronic recombination (DR) is a key atomic process that affects the spectroscopic diagnostic modeling of tungsten, most of whose ionization stages will be found somewhere in the ITER fusion reactor: in the edge, divertor, or core plasma. Accurate DR data are sparse while complete DR coverage is unsophisticated (e.g., average-atom or Burgess General Formula), as illustrated by the large uncertainties that currently exist in the tungsten ionization balance. To this end, we present a series of partial final-state-resolved and total DR rate coefficients for W^{73+} to W^{56+} tungsten ions. This is part of a wider effort within *The Tungsten Project* to calculate accurate dielectronic recombination rate coefficients for the tungsten isonuclear sequence for use in collisional-radiative modeling of finite-density tokamak plasmas. The recombination rate coefficients have been calculated with AUTOSTRUCTURE using κ-averaged relativistic wave unctions in level resolution (intermediate coupling) and configuration resolution (configuration average). Comparison with previous calculations of total DR rate coefficients for W^{63+} and W^{56+} yield agreement to within 20% and 10%, respectively, at peak temperature. It is also seen that the Jüttner correction to the Maxwell distribution has a significant effect on the ionization balance of tungsten at the highest charge states, changing both the peak abundance temperatures and the ionization fractions of several ions.

DOI: 10.1103/PhysRevA.93.042703

So… where are we now?

Partial and Total Dielectronic Recombination Rate Coefficients for W^{55+} to W^{38+}

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(Dated: September 28, 2016)

Censored!

So… where are we now?

- Ions $W^{73+} - W^{56+}$ (01-like – 18-like): now published.
- Ions $W^{55+} - W^{37+}$ (19-like – 36-like): Paper Submitted
- Ions $W^{36+} - W^{26+}$ (37-like – 46-like): MOSTLY finished, paper being written.
- Ions W^{26+} onwards: Mentally preparing ourselves.

Future work

- Continue calculations into 4f shell and beyond.
- Updated ionization balances with new data.
- Collisional-Radiative modelling - Plasma Emissivity et al.
- Effective ionization/recombination rate coefficients for transport codes.

W45+ Comparison