The Tungsten Project: Partial and Total Recombination rate coefficients for W^{74+} to W^{56+}

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About me

- Postdoctoral researcher at the University of Strathclyde, Glasgow.
- Supervised by Prof Nigel Badnell.
- Research interests include NTLE stellar atmospheres, particularly white dwarf atmospheres, spectroscopy, nuclear energy, and atomic data calculations.
- Currently funded by an EPSRC grant

The Tungsten Project

- Aim: To calculate detailed partial recombination rate coefficients for the entire tungsten isonuclear sequence, required for ADAS collisional-radiative modelling of finite density magnetic fusion plasma.

- We aim to cover the entire isonuclear sequence in configuration average within a year, followed by intermediate coupling calculations afterwards.

- Publish data in an open forum (OPEN-ADAS) in ADAS standard formats adf09 (dielectronic recombination) and adf48 (radiative recombination). Accompanied by input data files (adf27 and adf28).

OPEN-ADAS

Atomic Data and Analysis Structure

Re I (6145.8Å)

Freeform | Wavelength | Ion

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About OPEN-ADAS

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS).

ADAS is a computer program managed by the University of Strathclyde and made up of a consortium of over twenty members.

The OPEN-ADAS system enables non-members, with an interest in fusion and astrophysics, to download and use ADAS data.

More about OPEN-ADAS

Freeform search

Search

▸ Freeform search examples

Freeform search | Search by wavelength | Search by ion

5 March 2015 – Next ADAS Workshop

The 2015 workshop will be held in Catania, Sicily on 1-2 October. Read more

The OPEN-ADAS data classes

The data contained within ADAS is strictly organised and precisely formatted. There are over fifty distinct types of data file. The scope of OPEN-ADAS is targetted on and limited to the release and organisation of general user relevant data from the ADAS databases and the provision of code, subroutines and procedures to enable such users of OPEN-ADAS to read the released data. These data classes are given below.

FUNDAMENTAL CLASSES

ADF 01

Charge exchange cross sections

nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

ADF 04

Resolved specific ion data collections

Coefficient data for a given ion which includes spontaneous emission coefficients and electron impact collisional rates and other optional processes.

ADF 07

Electron impact ionisation coefficients

Collections of Maxwell averaged electron impact ionisation rate coefficients for both direct ionisation and excitation/autoionisation.

DERIVED CLASSES

ADF 11

Iso-nuclear master files

Effective (collisional–radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

ADF 12

Charge exchange effective emission coefficients

Collections of effective emission coefficients for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms.

ADF 13

Ionisation per photon coefficients

Data collections useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface.

Previous efforts

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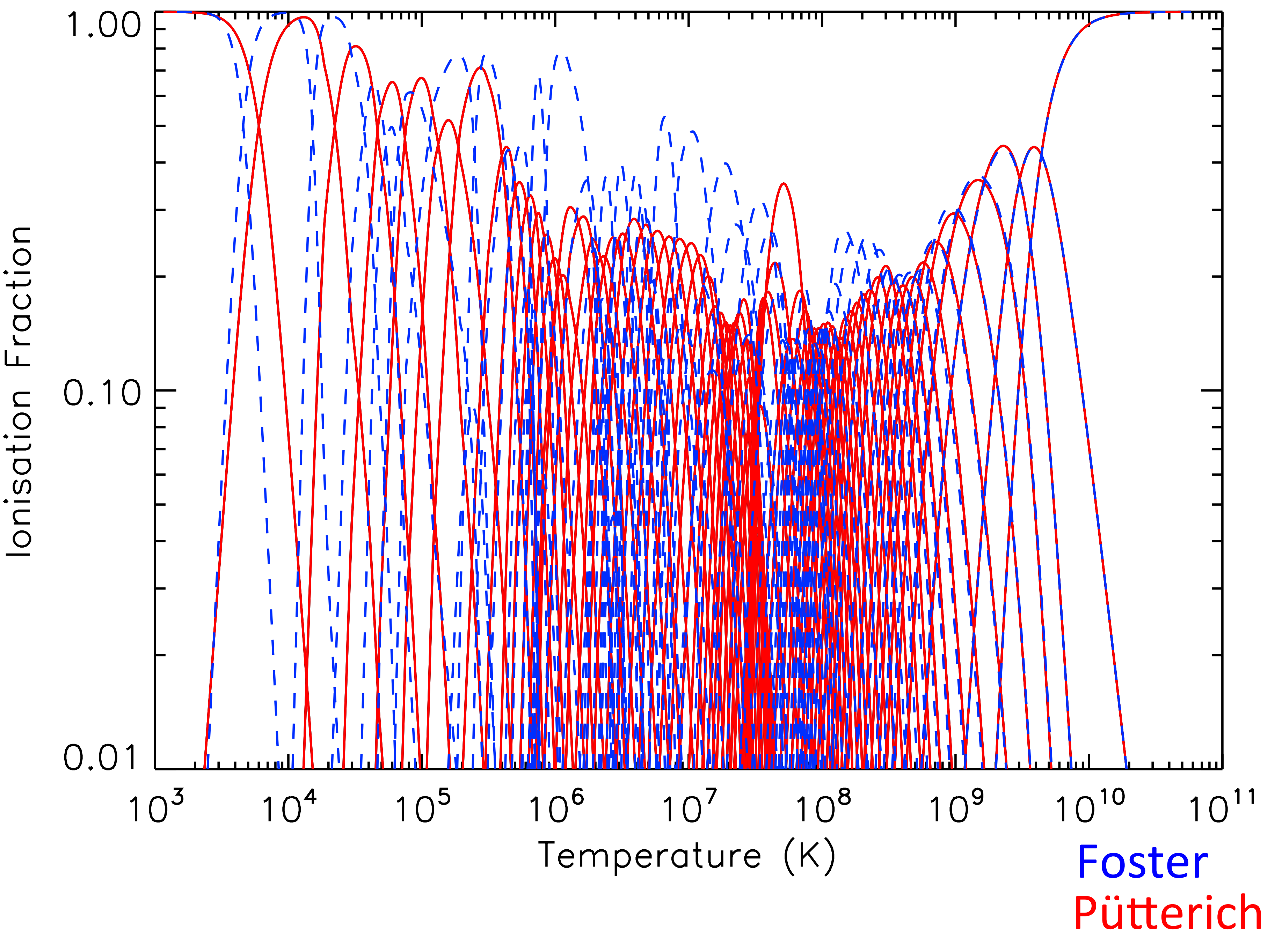
- Putterich (2008) calculated Recombination rate coefficients for the isonuclear sequence of Tungsten, using the average ion model.
- Quick to calculate, but neglects mixing and has poor resolution. Also provides totals only.
- Foster (2008) utilises a mix of the Burgess General Formula, and Burgess-Bethe General Program (BBGP).
- Using ionisation rate coefficients of Loch (2008), we can compare the ionisation balances of Putterich and Foster.


1.00
0.10
0.01
Ionisation Fraction
10^3
10^4
10^5
10^6
10^7
10^8
10^9
10^10
10^11
Temperature (K)
Foster
Pütterich

Previous efforts

- Agreement between Pütterich and Foster from Bare to Ne-like, where Radiative Recombination is dominant.

- Dielectronic Recombination steadily becomes more important as residual charge decreases.

- Discrepancy between Pütterich and Foster isn't limited to ionisation stage population, there is also a large discrepancy between peak abundance temperatures.

Previous efforts

- Individual ions have also been considered, mainly for closed sub-shell ions.

- Ne-like (Behar 1999, Safronova 2009), Na-like (Safronova 2009), and Ar-like (Peleg 1998), all calculated using HULLAC.

- Lower charge ions also considered include Pd and Er-like (Safronova 2011, Safronova 2012), and others presented in this meeting.

AUTOSTRUCTURE

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- General atomic structure/collision package (Badnell 1986, 1997, 2011) based on SUPERSTRUCTURE (Eissner 1974).
- Calculates energy levels, radiative and autoionisation rates, photoionisation cross sections and more.
- Interaction between DR/RR negligible (Pindzola 1992) - Independent Processes/Isolated Resonances Distorted Wave (IPIRDW) approach to DR (Badnell 2003). For the full coupled case, ask Connor Ballance!

AUTOSTRUCTURE

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- Kappa-averaged relativistic wavefunctions.
- Level Resolved - Intermediate Coupling (IC), Term Resolved (LS), and configuration resolved - Configuration Average (CA). Terms/Levels can be further 'bundled'.
- Simple, user friendly input.
- Cross sections have been compared to experimental results such as the TSR storage ring in Heidelberg. W^{20+} IC DR rates come within 20% for T_e<2eV.
- Comparisons with W^{18+} yield closer agreement.

File Edit Options Buffers Tools Help

```
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3 0 3 1 3 2
 2 2 0          N-electron ground plus excitations
 2 1 1
 1 3 0
 1 2 1
 0 4 0          Mixing
 2 0 2          Mixing

 2 3 0          N+1-electron ground
 2 2 1
 2 1 2
 1 4 0
 1 3 1
 1 2 2
 0 5 0
 0 4 1
 2 0 3
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C-------------------------------------------------------------------------------
C  AUTOSTRUCTURE input file for adf09 dielecronic recombination rate calculation
C  Base file for Delta n=0, 2-2 core excitation.
C
C  Producer : Simon P Preval
C  Date     : 24-01-15
C-------------------------------------------------------------------------------
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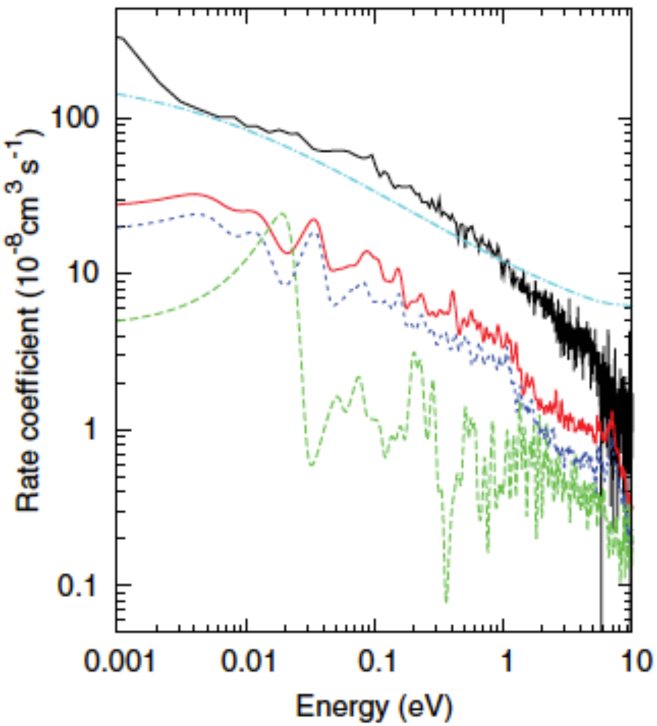

FIG. 5. (Color online) W^{20+} merged-beam DR rate coefficients: experiment [7] [upper solid (black) curve], partitioned total [dot-dashed (cyan) curve], IC total [lower solid (red) curve], *LS* total [long-dashed (green) curve], and IC $4d \rightarrow 4f$ only [short-dashed (blue) curve].

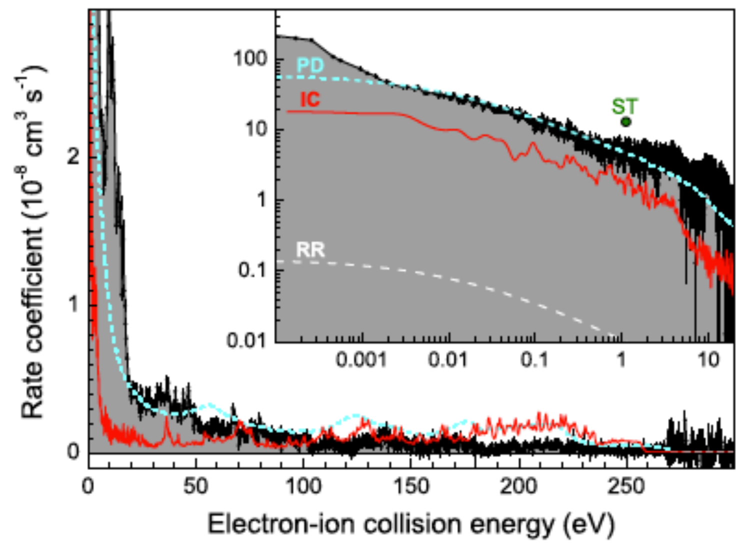

FIG. 3. (Color online) Comparison of our measured (symbols) and various calculated merged-beam recombination rate coefficients. The solid curve (labeled IC) is the result of the present intermediate-coupling calculation. The short-dashed curve (labeled PD) is the result of the fully partitioned calculation 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+

DR Rate Coefficients

- Dominant core excitations determined by running cases in CA, and checking each excitations' contribution to the total DR rate coefficient.

- Contributions calculated up to N=25 sequentially, and then logarithmically up to N=999. L calculated such that total DR rate coefficients converged to <1%.

- N-electron configurations consist of the ground plus single electron excitations, first excited configuration plus single electron excitations, plus any mixing configurations. Additional N+1-electron configurations allow for Rydberg radiation.

DR Rate Coefficients

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Ion	Core Excitations (n_i –> n_f)	Ion	Core Excitations (n_i –> n_f)
W73+ (H-like)	1 – 2, 1 – 3	W64+ (Ne-like)	2 – 3, 2 – 4
W72+ (He-like)	1 – 2, 1 – 3	W63+ (Na-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W71+ (Li-like)	1 – 2, 2 – 2, 2 – 3, 2 – 4	W62+ (Mg-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W70+ (Be-like)	1 – 2, 2 – 2, 2 – 3, 2 – 4	W61+ (Al-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W69+ (B-like)	2 – 2, 2 – 3	W60+ (Si-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W68+ (C-like)	2 – 2, 2 – 3	W59+ (P-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W67+ (N-like)	2 – 2, 2 – 3	W58+ (S-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W66+ (O-like)	2 – 2, 2 – 3	W57+ (Cl-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5
W65+ (F-like)	2 – 2, 2 – 3	W56+ (Ar-like)	2 – 3, 3 – 3, 3 – 4, 3 – 5

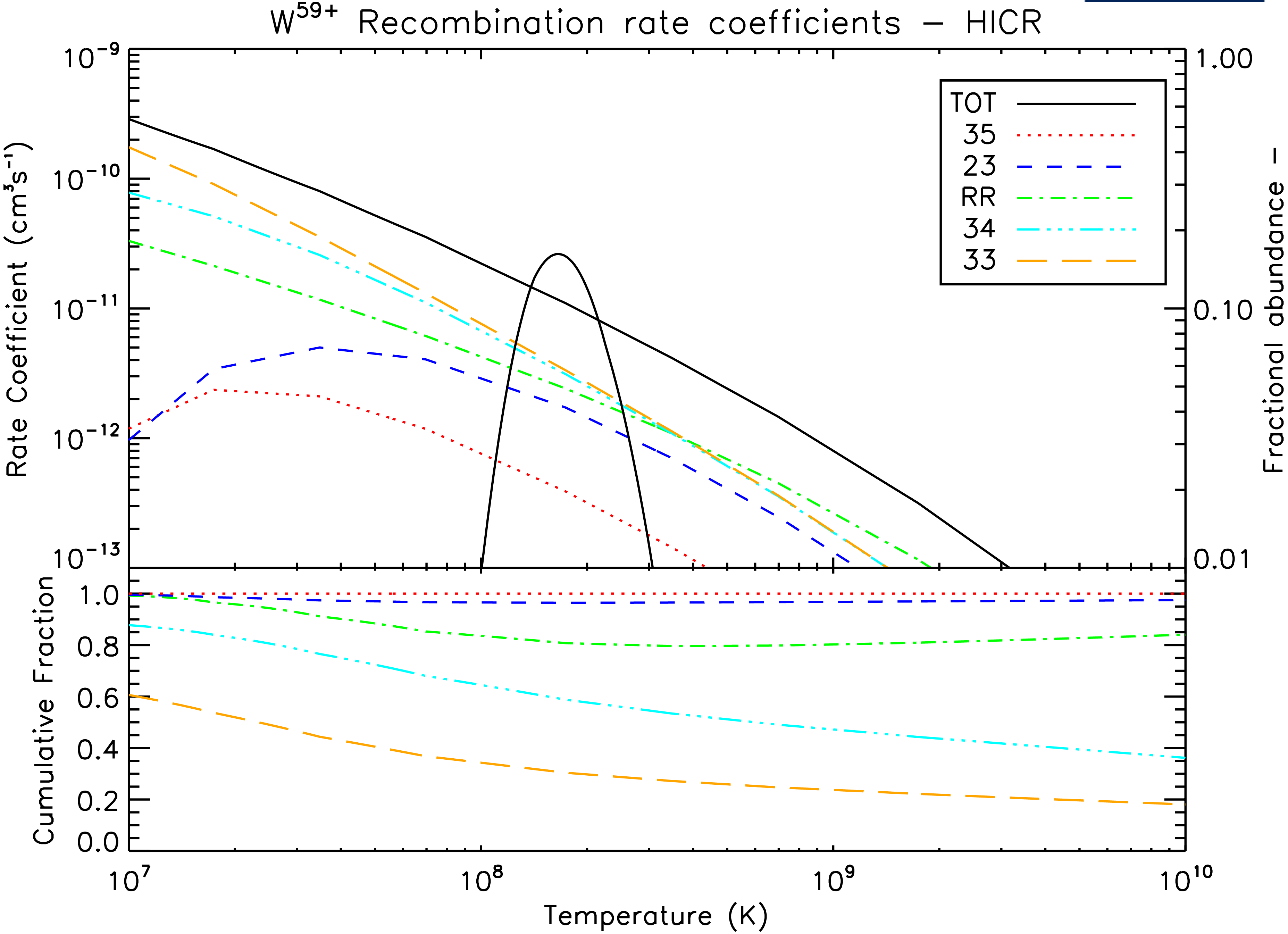
Redacted.

RR Rate Coefficients

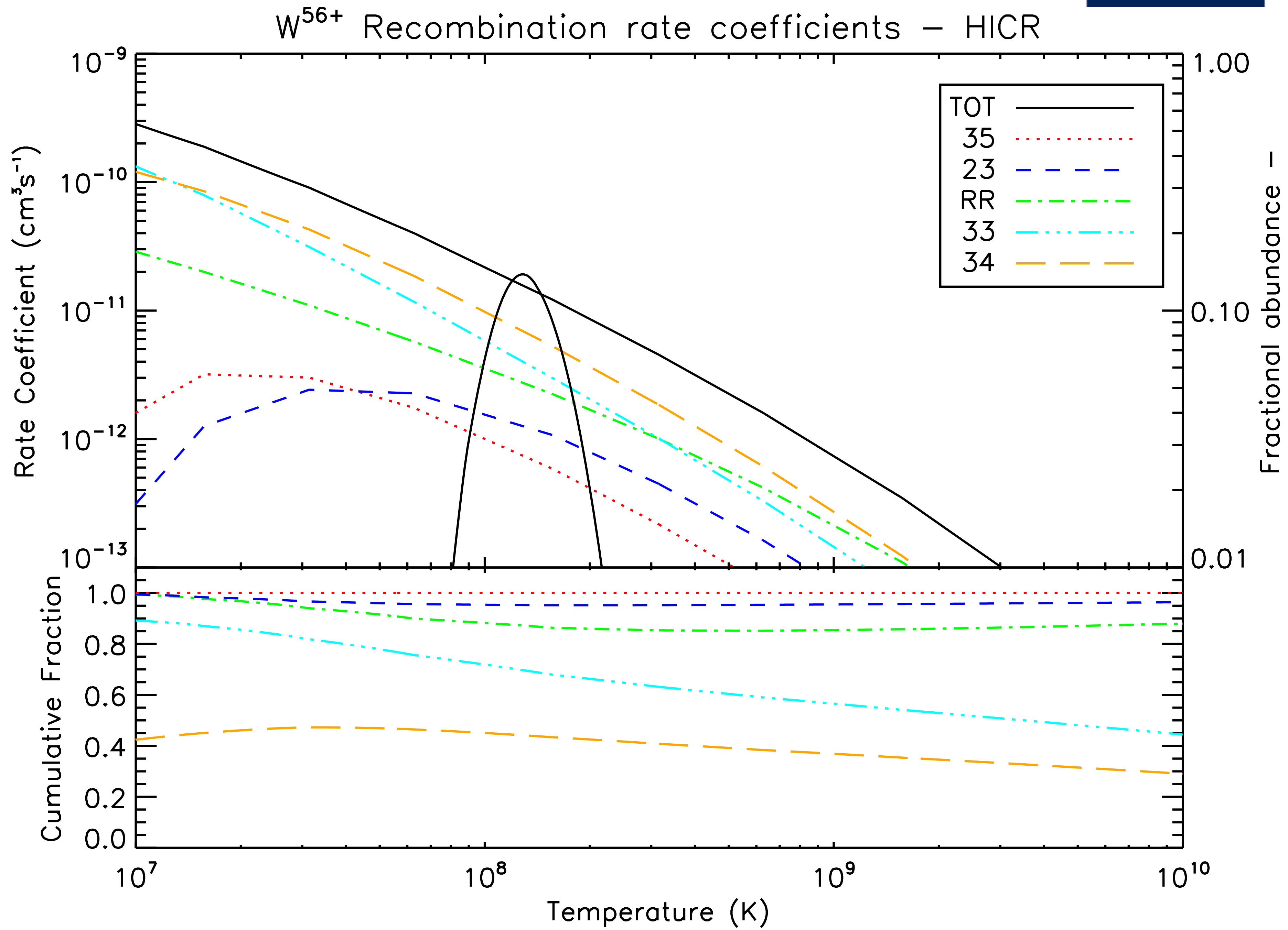
- Contributions calculated up to N=25 sequentially, then up to N=999 logarithmically. L calculated up to L=10 relativistically, then up to L=150 as a non-relativistic top up.

- Multipole contributions up to E40 and M39.

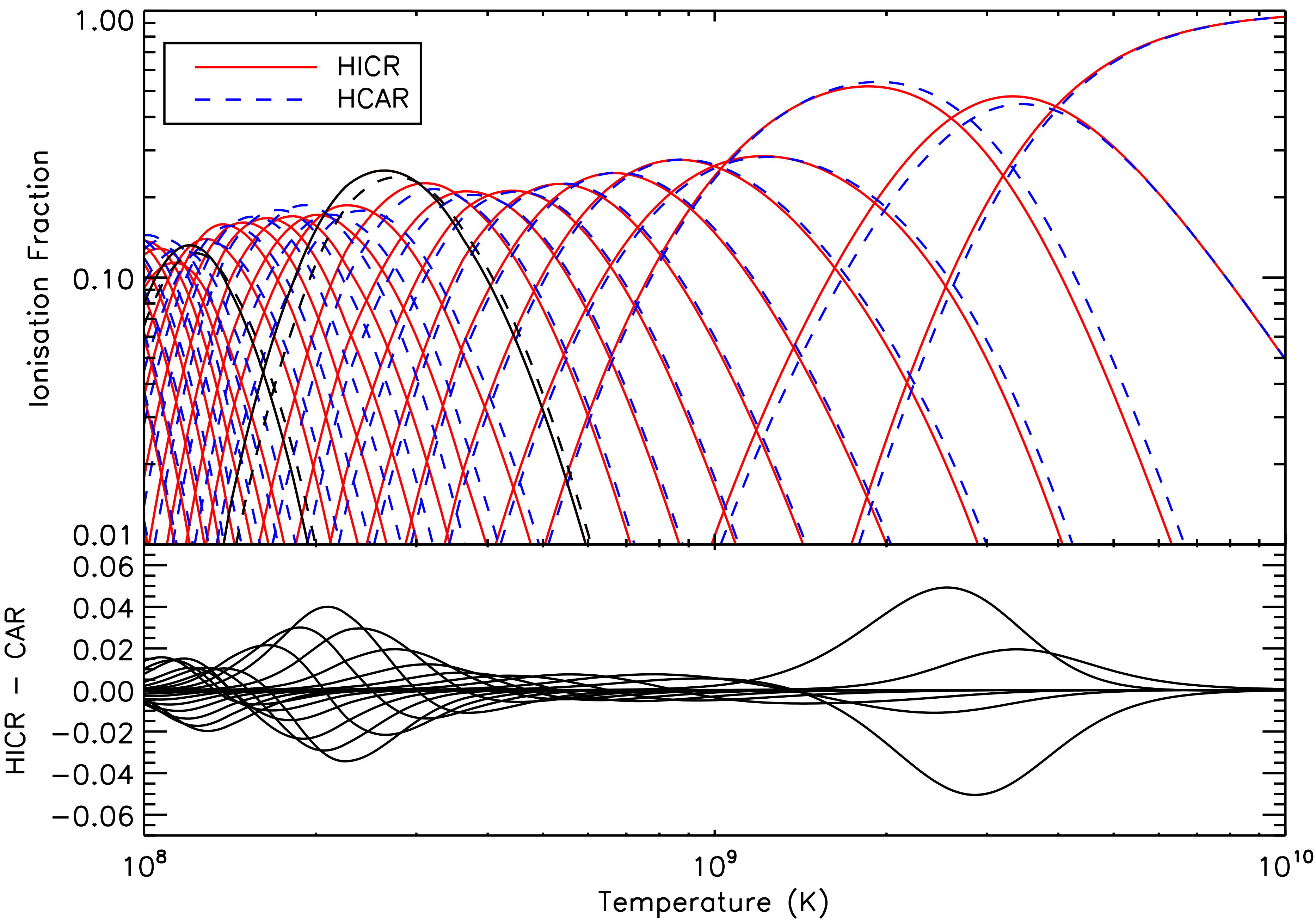
- Configurations included are just a subset of the DR ones.



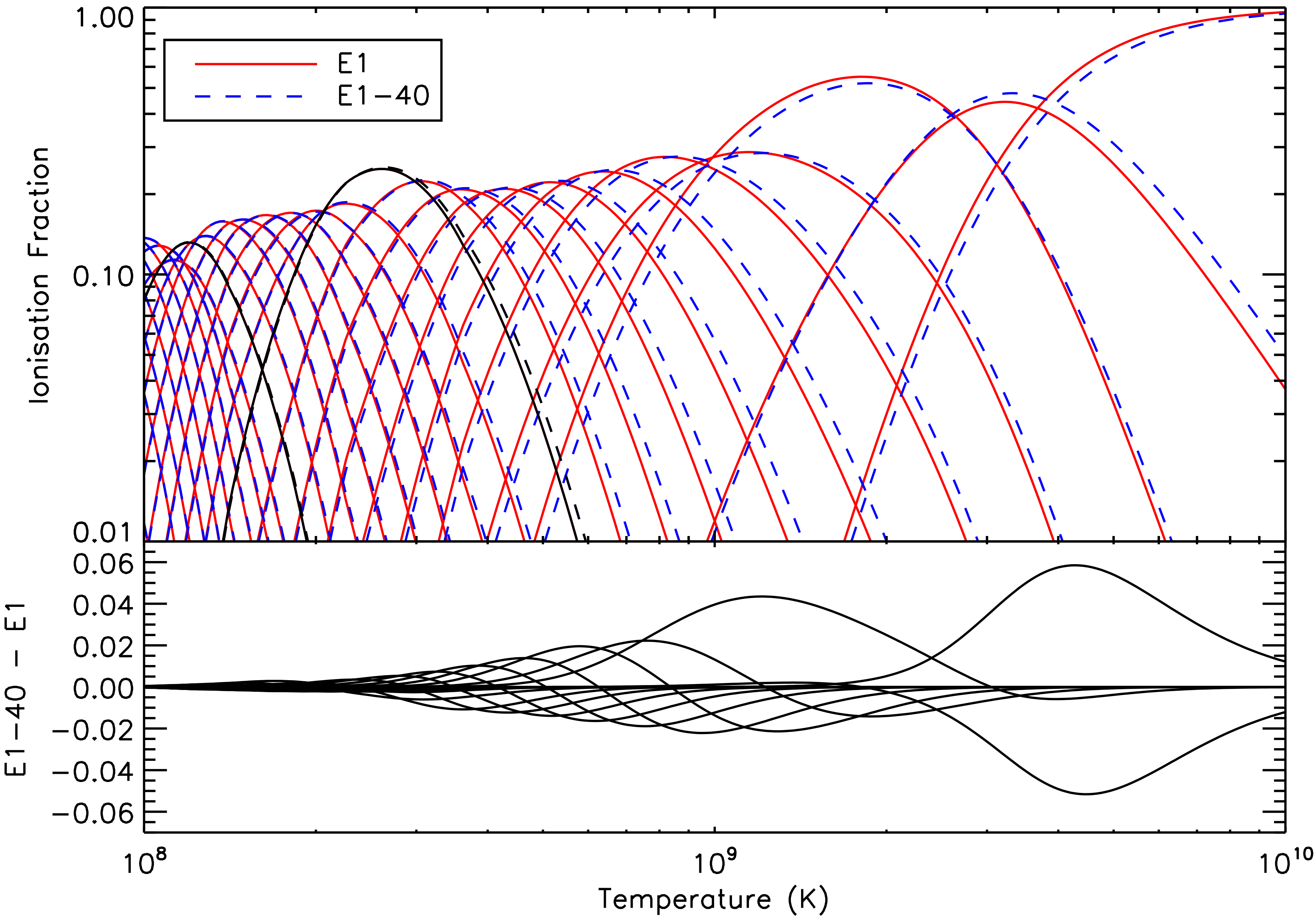
W59+ Recombination rate coefficients – HICR
TOT
35
23
RR
34
33
Rate Coefficient (cm3s-1)
Fractional abundance –
Cumulative Fraction
Temperature (K)
10-9
10-10
10-11
10-12
10-13
1.00
0.10
0.01
1.0
0.8
0.6
0.4
0.2
0.0
107
108
109
1010



W56+ Recombination rate coefficients – HICR
Rate Coefficient (cm3s-1)
Fractional abundance –
Cumulative Fraction
Temperature (K)
TOT
35
23
RR
33
34
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
1010



HICR
HCAR
1.00
0.10
0.01
Ionisation Fraction
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
HICR − CAR
10^8
10^9
10^{10}
Temperature (K)

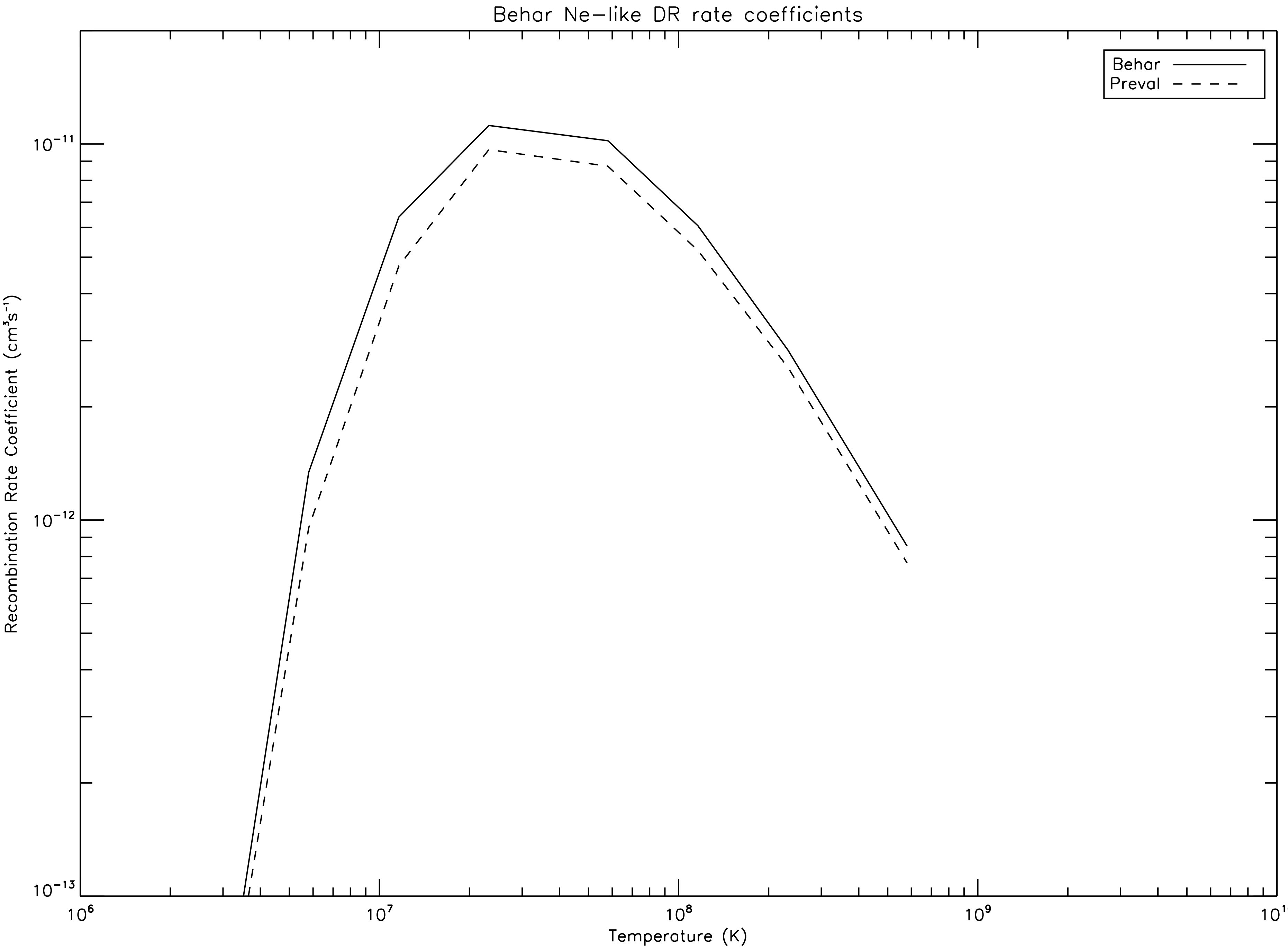

E1
E1−40
Ionisation Fraction
1.00
0.10
0.01
E1−40 − E1
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
10^8
10^9
10^{10}
Temperature (K)

Comparisons

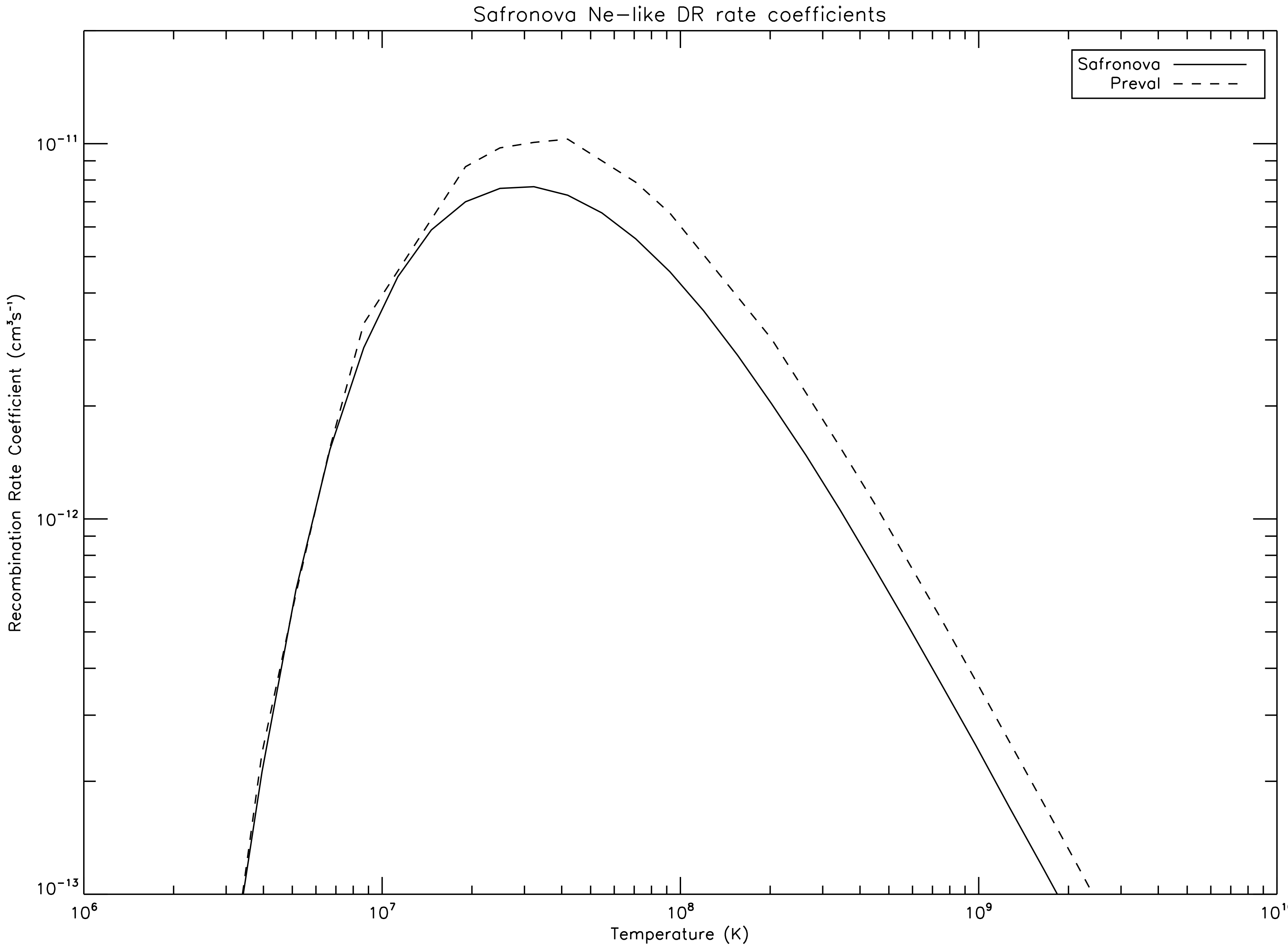
- Detailed DR rate coefficient calculations (tabulated) exist for Ne (Behar 1999, Safronova 2009) and Ar-like (Peleg 1998) tungsten, all calculated using HULLAC.

- Behar rates and ours agree to < 20% for Te > 2E+07K. Agreement significantly worse for Safronova rates. ~50% for Te > 2E+08K, but this is improved by ~10% if we remove 2-4 core excitation.

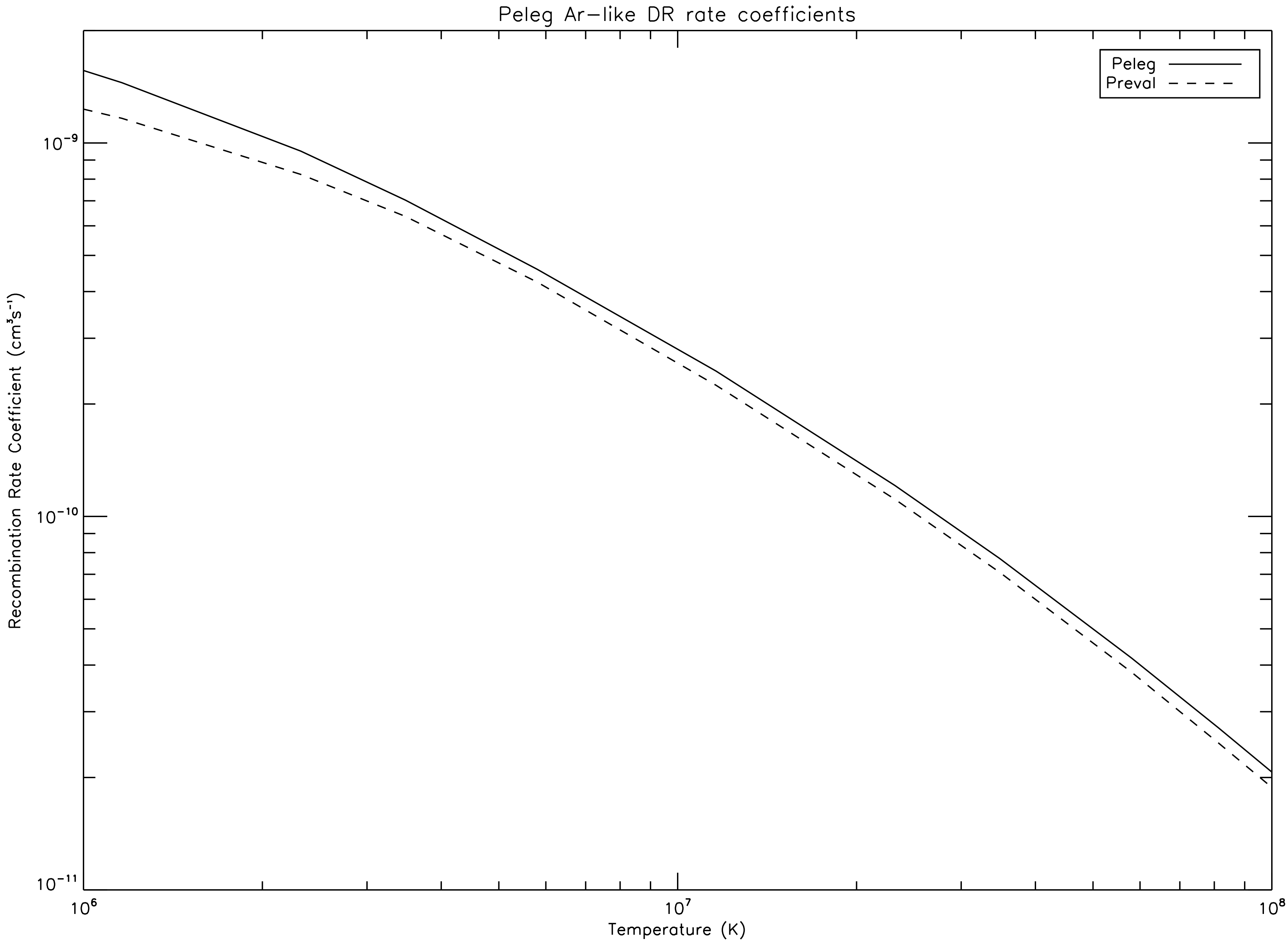
- Best agreement between our rates and Peleg. < 10% for Te > 3E+06K.



Behar Ne−like DR rate coefficients
Behar
Preval
Recombination Rate Coefficient (cm³s⁻¹)
Temperature (K)
10^{-11}
10^{-12}
10^{-13}
10^{6}
10^{7}
10^{8}
10^{9}
10^{10}



Safronova Ne-like DR rate coefficients
Safronova
Preval
Recombination Rate Coefficient (cm³s⁻¹)
Temperature (K)
10⁻¹¹
10⁻¹²
10⁻¹³
10⁶
10⁷
10⁸
10⁹
10¹⁰

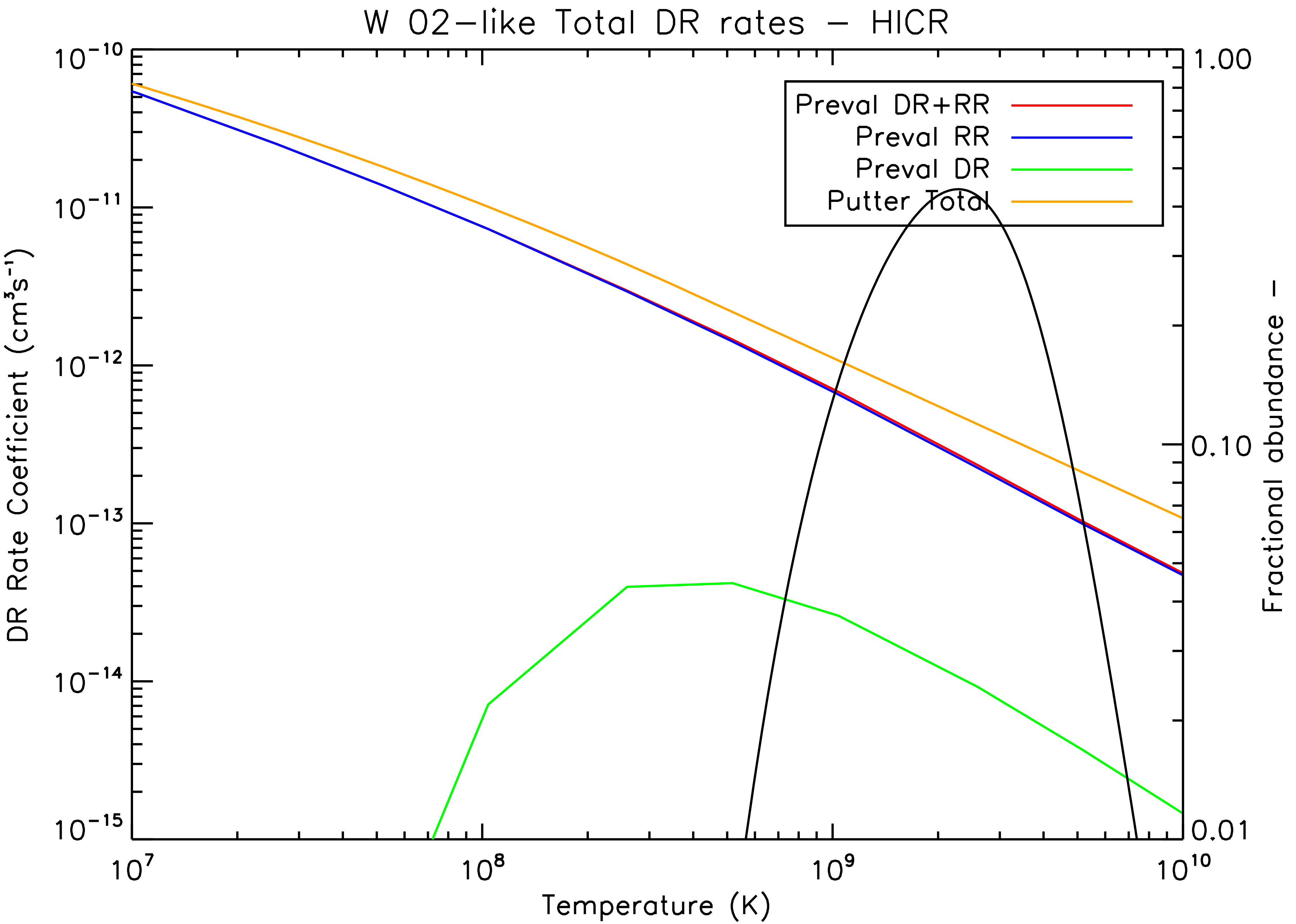

Peleg Ar–like DR rate coefficients
Peleg
Preval
Recombination Rate Coefficient (cm³s⁻¹)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁶
10⁷
10⁸
Temperature (K)

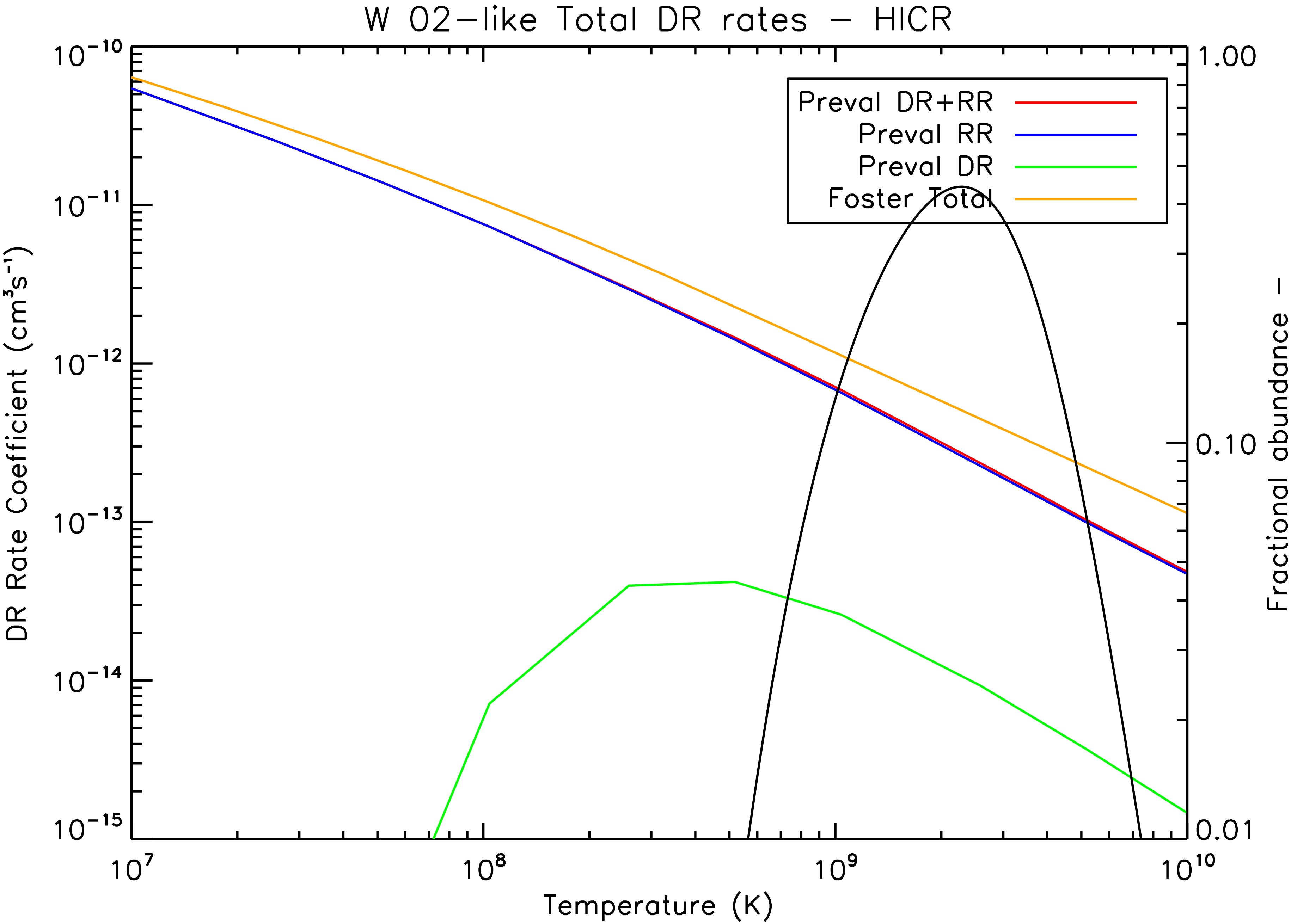
Comparisons

- Putterich and Foster only provides totals for their recombination rates.

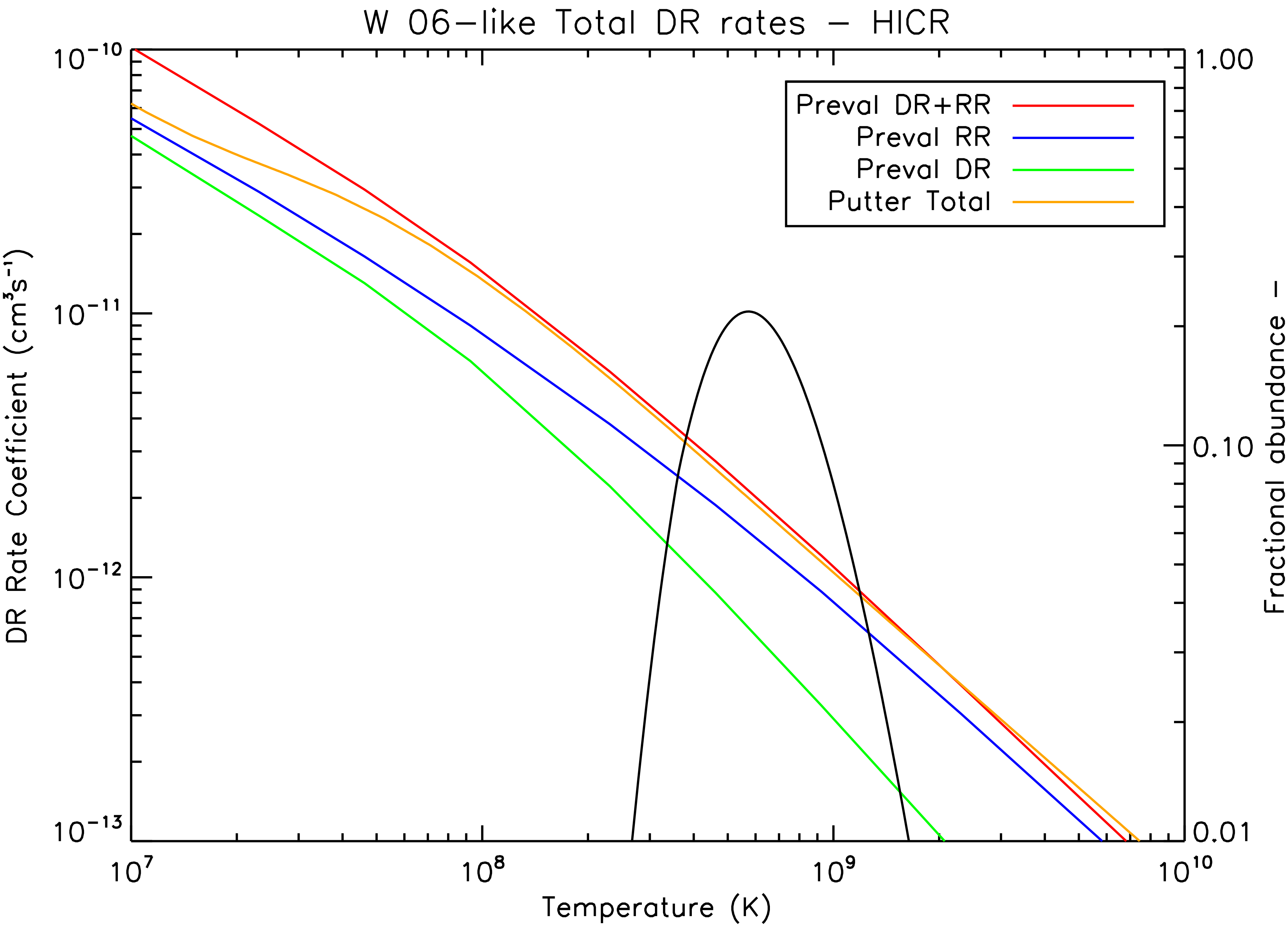
- Putterich and Foster rate totals in good agreement for half-filled shells. This quickly deteriorates for closed subshell ions.

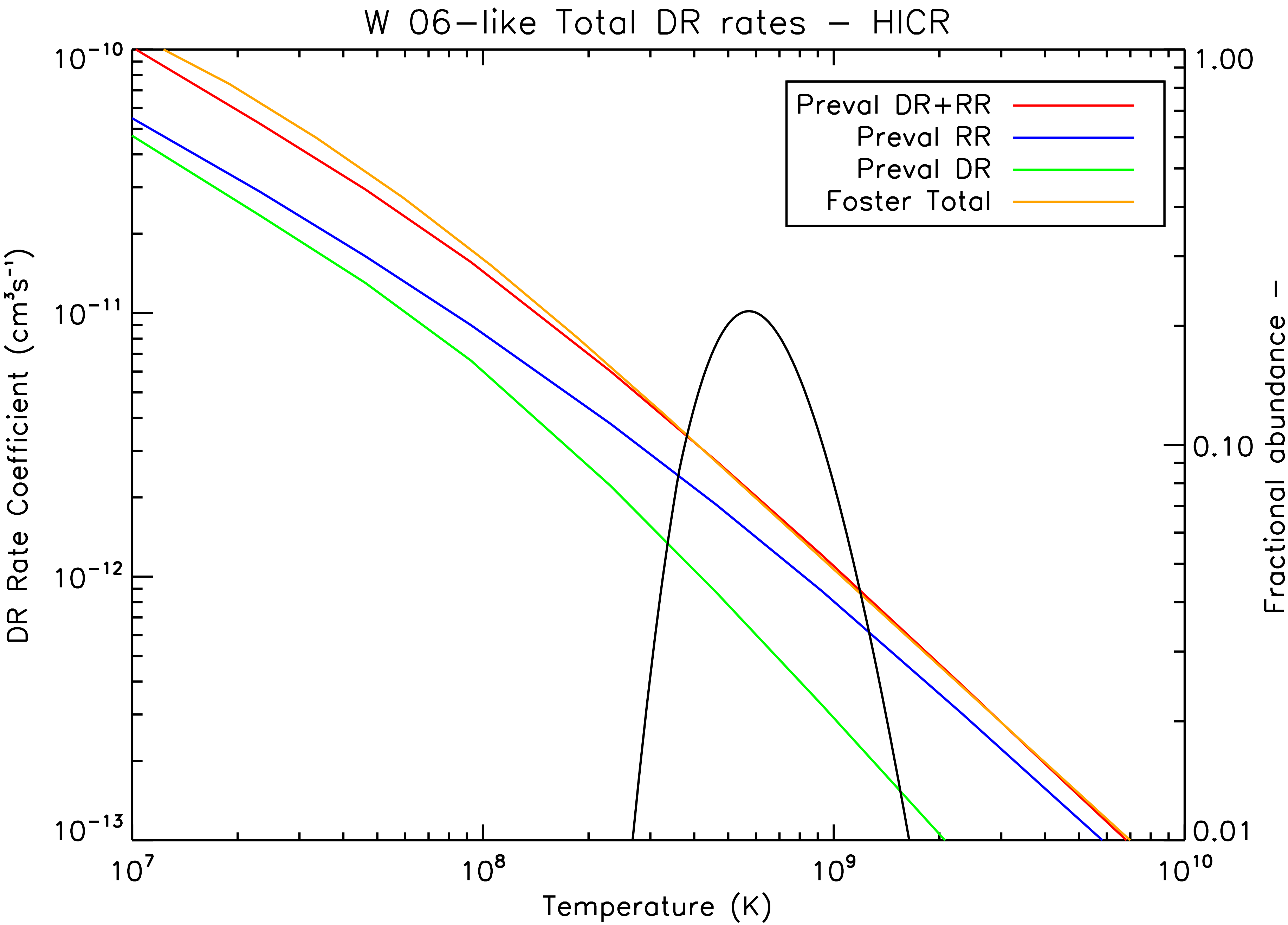
- Best agreement <1% for C-like. Worst agreement in He-like, >100% in places!

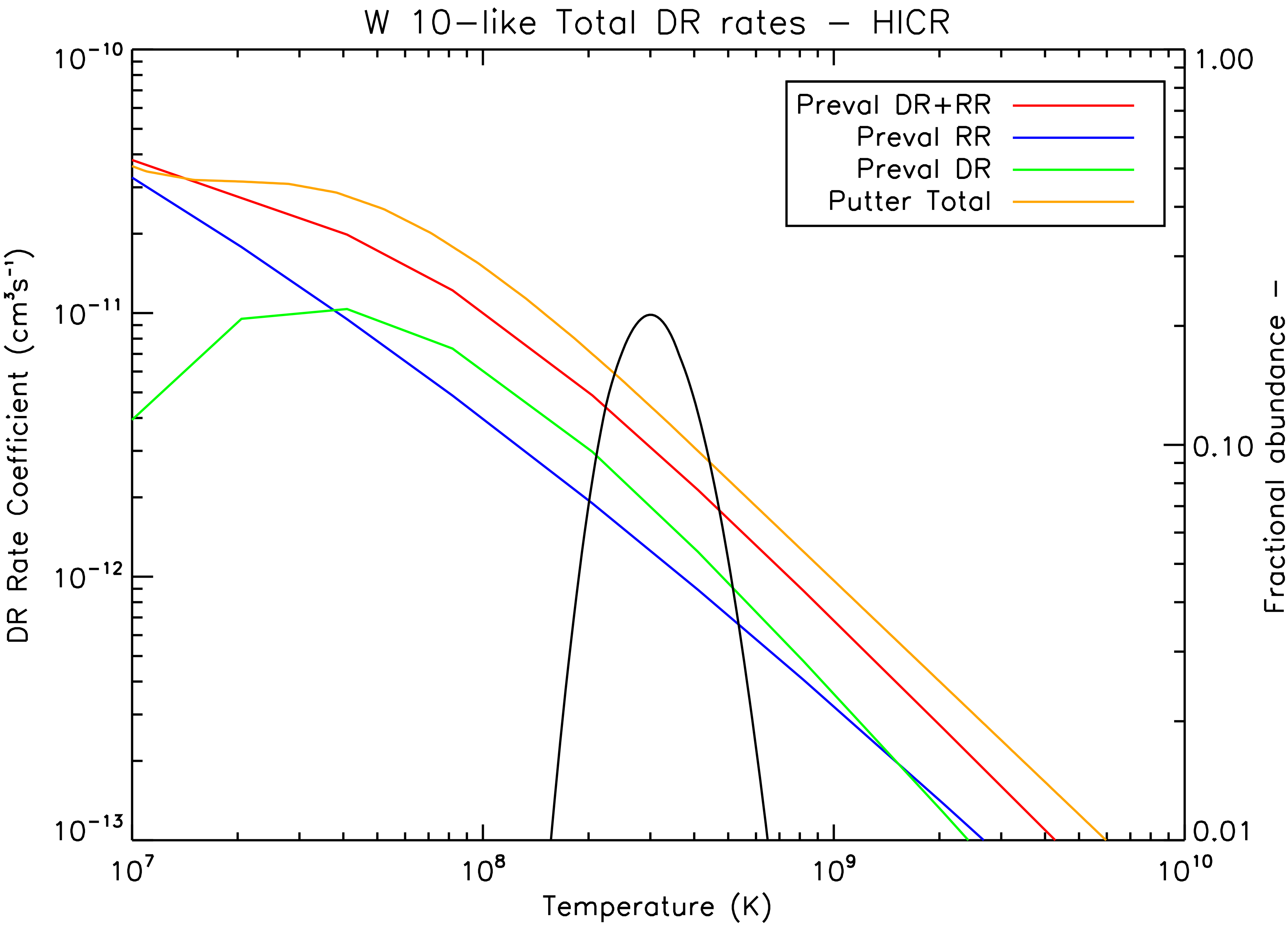

W 02-like Total DR rates - HICR
DR Rate Coefficient (cm^{3}s^{-1})
Fractional abundance -
Temperature (K)
Preval DR+RR
Preval RR
Preval DR
Putter Total
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
1.00
0.10
0.01
10^{7}
10^{8}
10^{9}
10^{10}



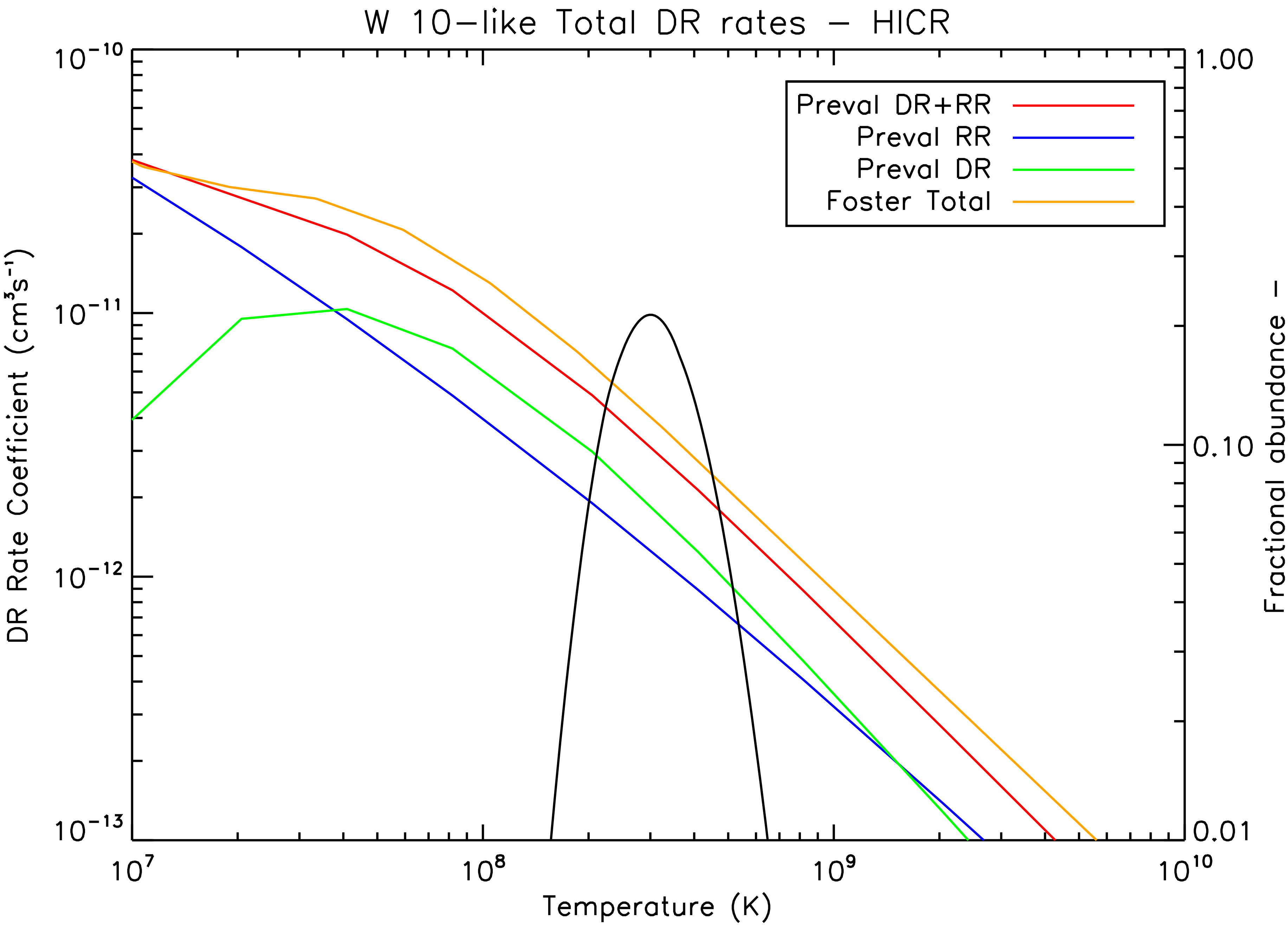
W 02-like Total DR rates - HICR
Preval DR+RR
Preval RR
Preval DR
Foster Total
DR Rate Coefficient (cm^{3}s^{-1})
Fractional abundance -
Temperature (K)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^7
10^8
10^9
10^{10}
1.00
0.10
0.01


W 06-like Total DR rates – HICR
Preval DR+RR
Preval RR
Preval DR
Putter Total
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance –
Temperature (K)
10⁻¹⁰
10⁻¹¹
10⁻¹²
10⁻¹³
1.00
0.10
0.01
10⁷
10⁸
10⁹
10¹⁰

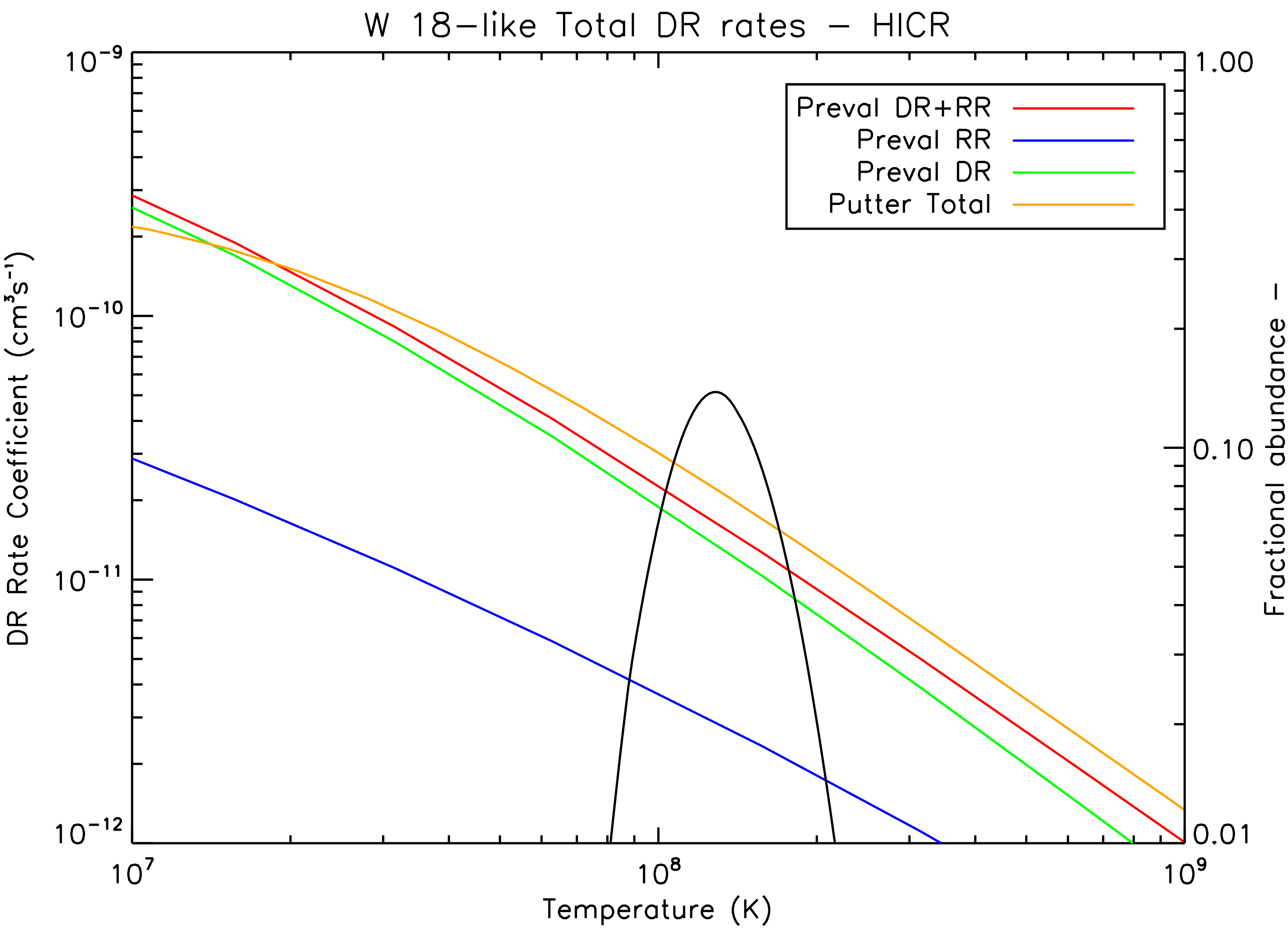

W 06-like Total DR rates - HICR
Preval DR+RR
Preval RR
Preval DR
Foster Total
DR Rate Coefficient (cm^3s^{-1})
Fractional abundance -
Temperature (K)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{7}
10^{8}
10^{9}
10^{10}
1.00
0.10
0.01



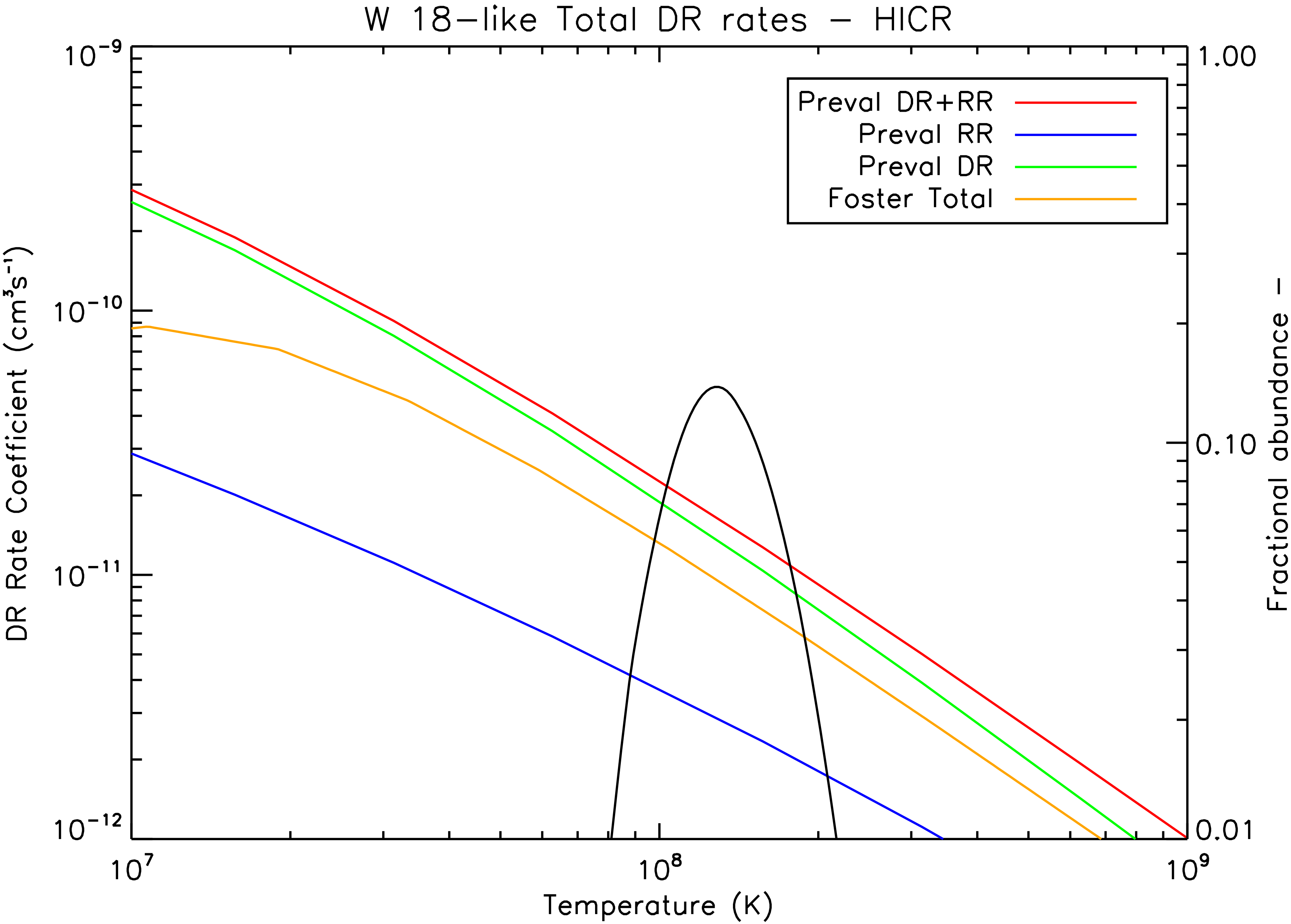
W 10-like Total DR rates - HICR
Preval DR+RR
Preval RR
Preval DR
Putter Total
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance -
Temperature (K)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
1.00
0.10
0.01
10^{7}
10^{8}
10^{9}
10^{10}



W 10-like Total DR rates - HICR
Preval DR+RR
Preval RR
Preval DR
Foster Total
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance -
Temperature (K)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
1.00
0.10
0.01
10^{7}
10^{8}
10^{9}
10^{10}



W 18-like Total DR rates – HICR
Preval DR+RR
Preval RR
Preval DR
Putter Total
DR Rate Coefficient (cm^{3}s^{-1})
Fractional abundance –
Temperature (K)
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^7
10^8
10^9
1.00
0.10
0.01

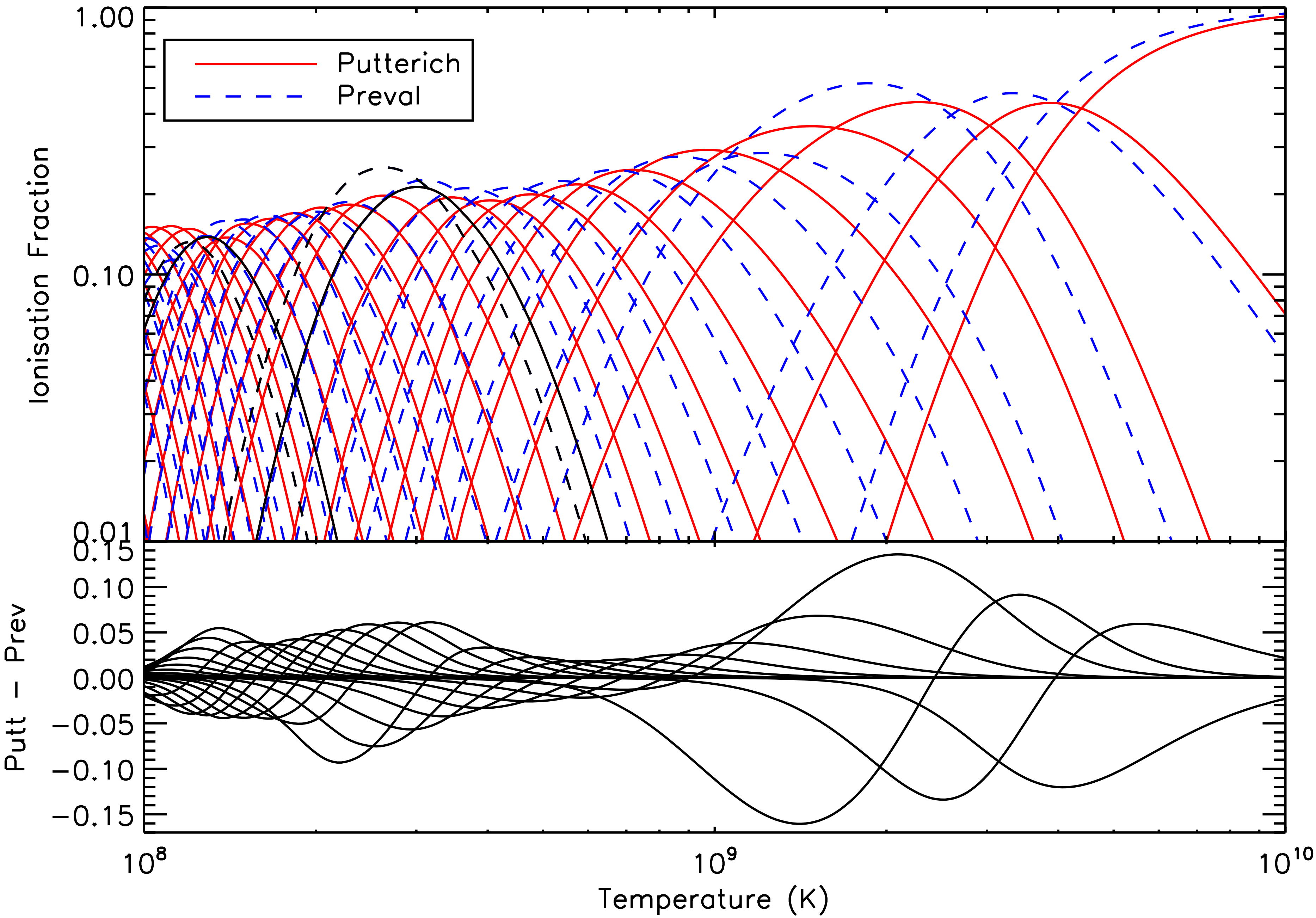


W 18-like Total DR rates - HICR
Preval DR+RR
Preval RR
Preval DR
Foster Total
DR Rate Coefficient (cm³s⁻¹)
Fractional abundance -
Temperature (K)
10⁻⁹
10⁻¹⁰
10⁻¹¹
10⁻¹²
1.00
0.10
0.01
10⁷
10⁸
10⁹

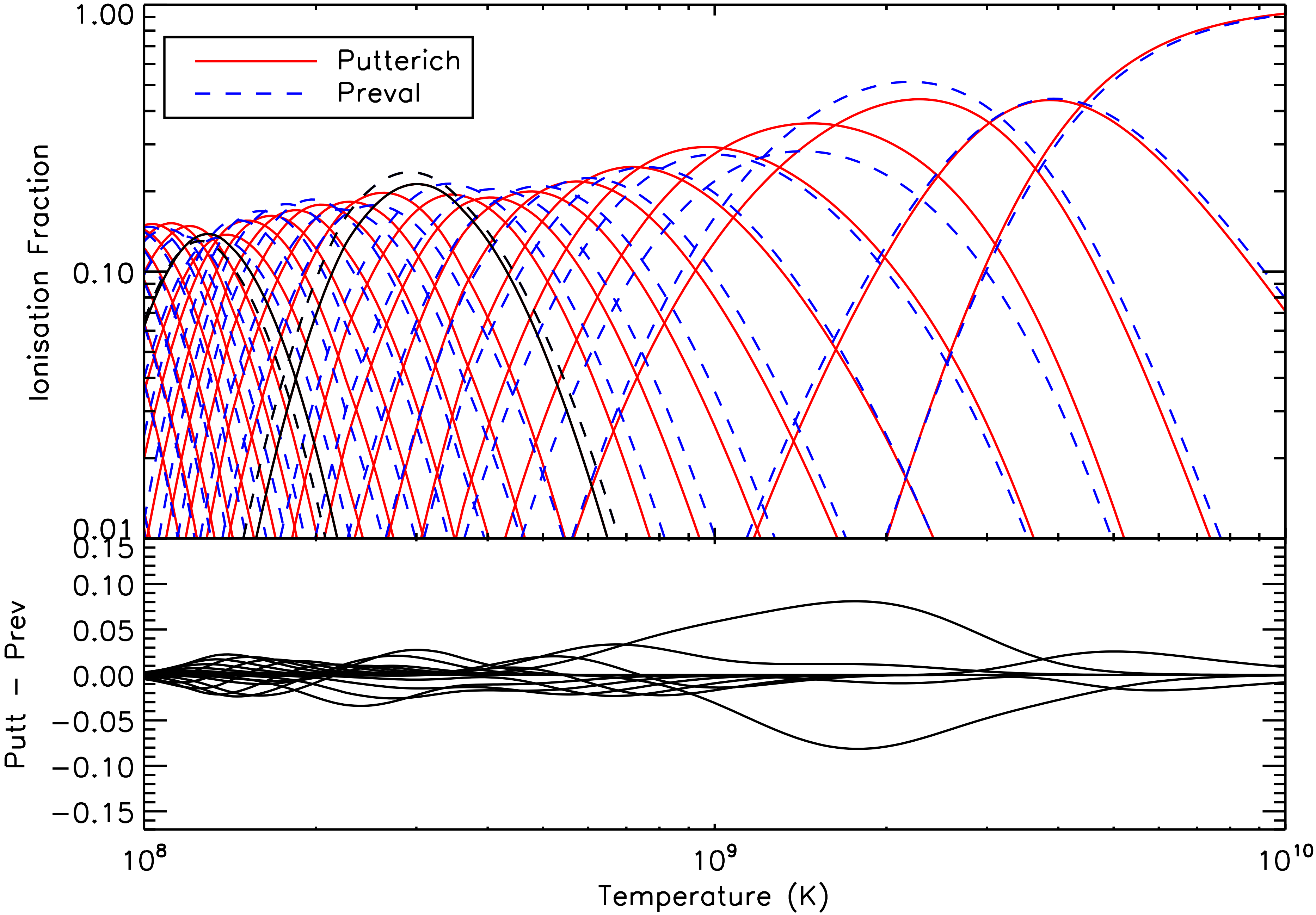
Comparisons

- To compare our ionisation balance with Putterich, we use the Putterich recombination data, but replace the relevant ions with our data.

- Calculated ionisation balance appears to be in good agreement with that of Putterich, provided we do not include the Juttner correction to the Maxwell distribution.



Putterich
Preval
Ionisation Fraction
1.00
0.10
0.01
Putt - Prev
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
10^8
10^9
10^{10}
Temperature (K)

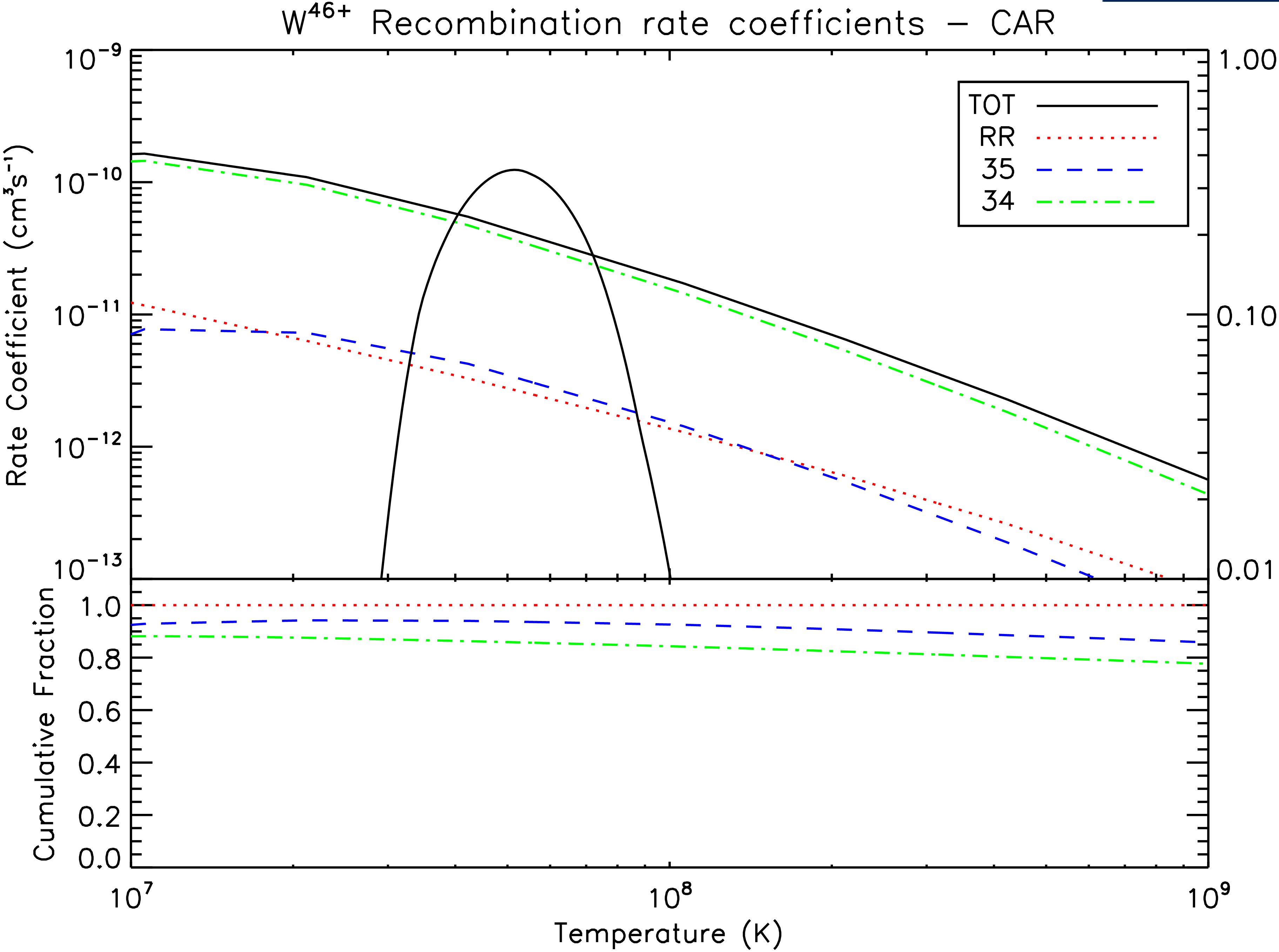


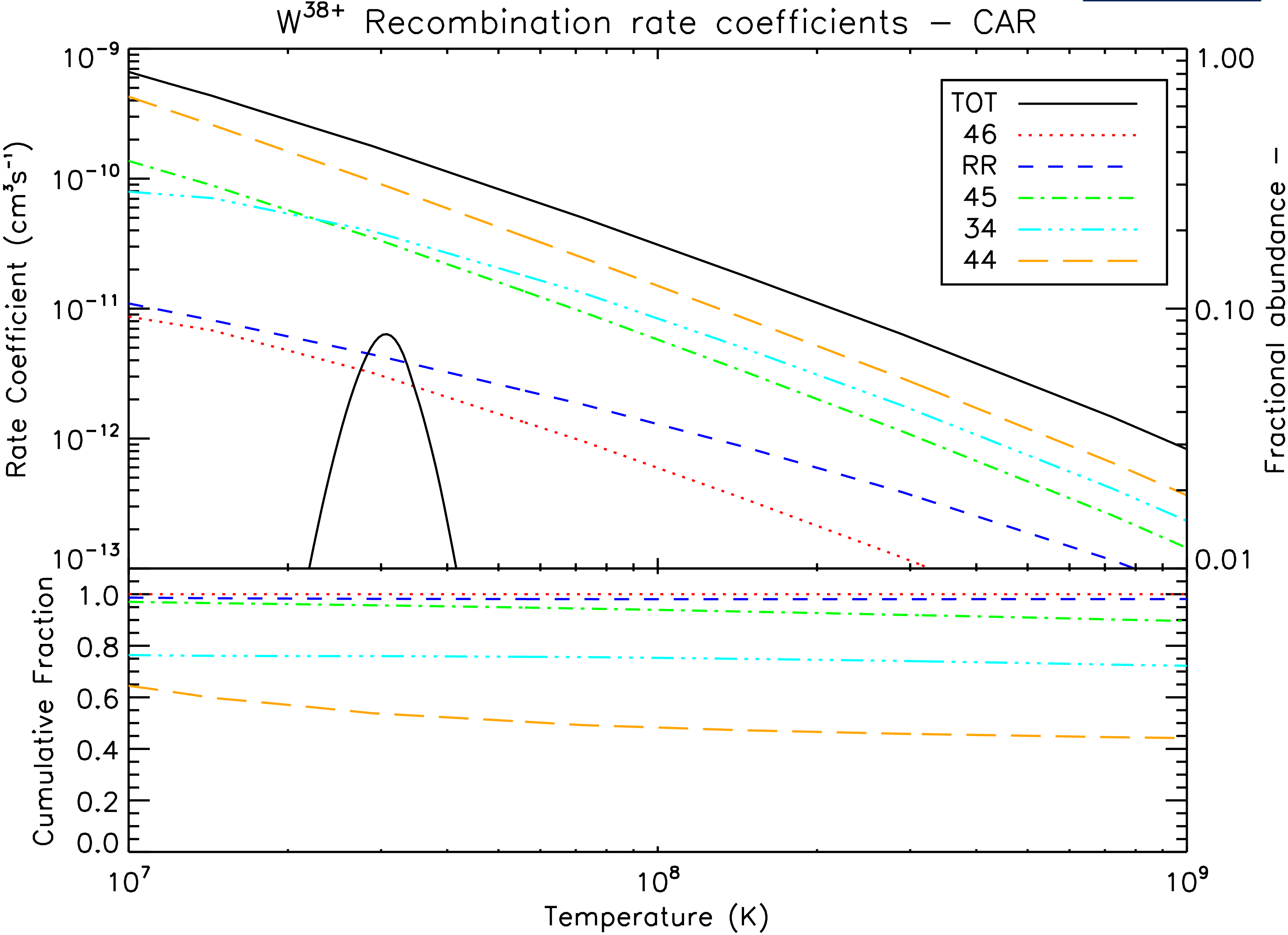
Putterich
Preval
Ionisation Fraction
1.00
0.10
0.01
Putt – Prev
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
10^8
10^9
10^{10}
Temperature (K)

Current Progress

- Officially, ions from bare-like to Ar-like have been calculated for all relevant core excitations in LS, IC, and CA.

- Unofficially, ions from K-like to Kr-like have also been calculated, but in CA only. Preparing to calculate these in intermediate coupling.


W46+ Recombination rate coefficients – CAR
TOT
RR
35
34
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



W^{38+} Recombination rate coefficients – CAR
Rate Coefficient (cm^{3}s^{-1})
Fractional abundance –
TOT
46
RR
45
34
44
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
1.00
0.10
0.01
Cumulative Fraction
1.0
0.8
0.6
0.4
0.2
0.0
10^7
10^8
10^9
Temperature (K)

Conclusions

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- We have presented "The Tungsten Project", and our aim of calculating partial DR rate coefficients for the isonuclear sequence of tungsten.
- We have covered W74+ to W56+ in intermediate coupling and configuration average.
- We have also gone further, and covered W55+ to W38+ in configuration average. We plan to cover the rest of the isonuclear sequence within the year.
- First publication due shortly!