Improvement and benchmarking of atomic data for kilonova modeling

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LABORATÓRIO DE INSTRUMENTAÇÃO
E FÍSICA EXPERIMENTAL DE PARTÍCULAS
partículas e tecnologia

Ciências ULisboa
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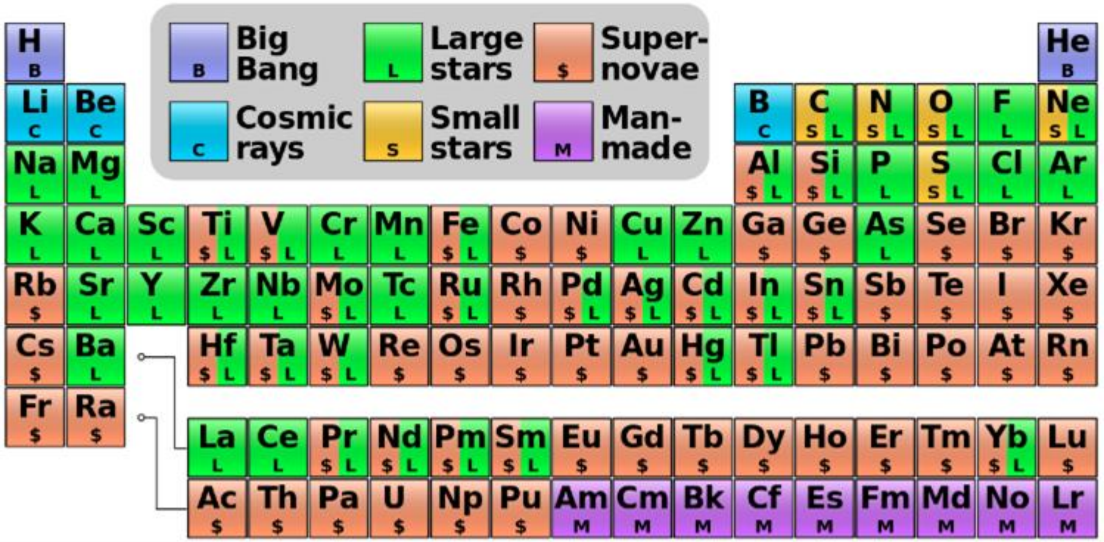
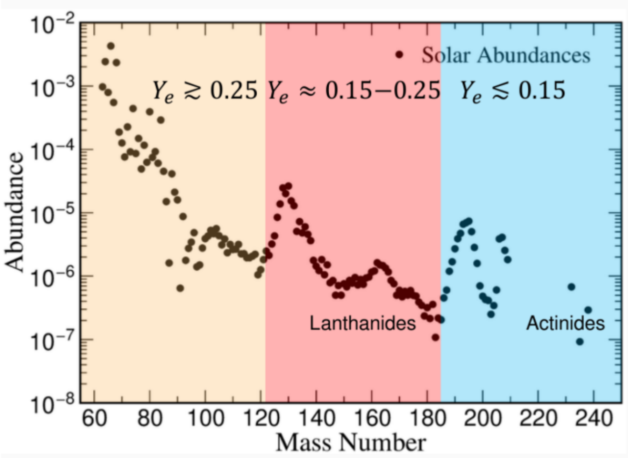
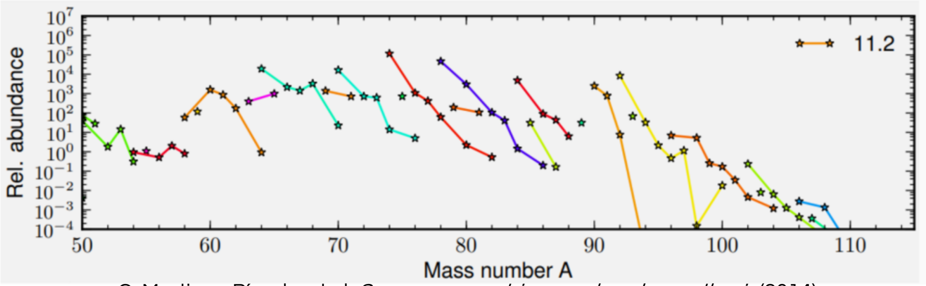
Motivation: Supernovae





$$Y_e = \frac{n_p}{n_p + n_n}$$

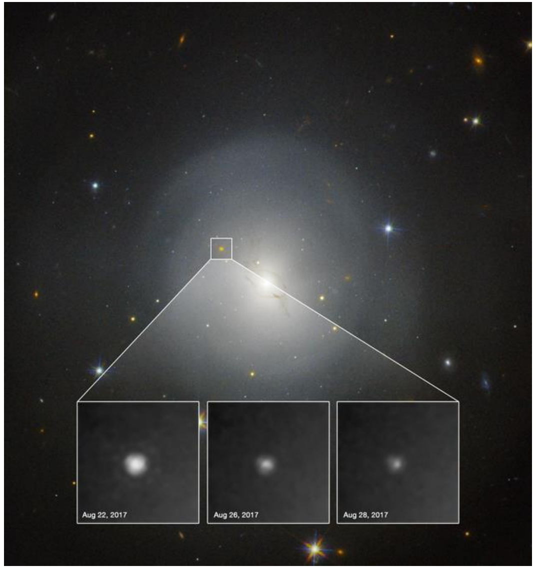
- Supernovae was thought to be the origin of the heavier elements;
- Electron fraction above the necessary to produce lanthanides and actinides.

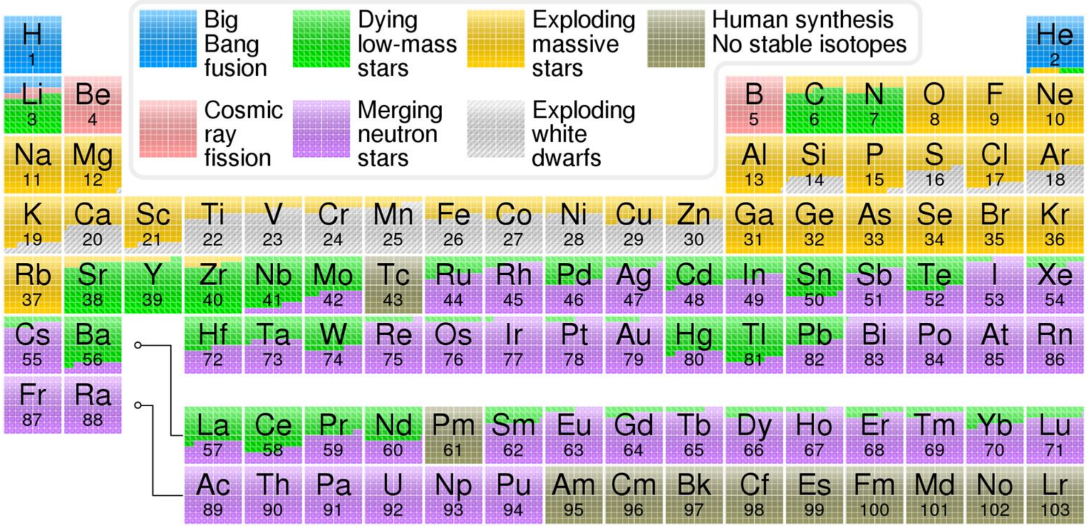


G. Martinez-Pínedo. et al, *Supernova neutrinos and nucleosynthesis* (2014)

Motivation: Kilonovae

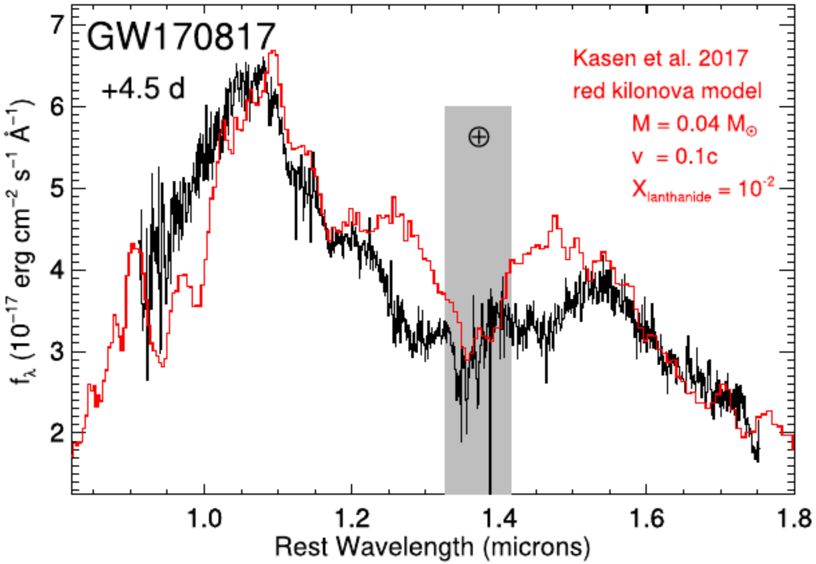
- In 2017 was observed the first kilonova after the neutron star merger GW170817.





- Initially there was almost no data for lanthanides and actinides:
  - Extremely complex;
  - No need in the atomic community until recently.

Motivation: Kilonovae



- First simulations used iron-peak elements:
  - Wrong conclusions because lanthanides and actinides have much higher number of levels/lines.

$$\mathcal{L} \approx 5 \times 10^{40}\,\mathrm{erg\,s^{-1}} \times \left(\frac{M}{0.01 M_\odot}\right)^{1-\frac{\alpha}{2}} \left(\frac{v_{ej}}{0.1c}\right)^{\frac{\alpha}{2}} \left(\frac{\kappa}{1\ \mathrm{cm^2\ g^{-1}}}\right)^{-\frac{\alpha}{2}}$$

Opacity → Encoding elemental abundances

METHOD - FAC

For the atomic data calculations we make extensive use of the FAC software package:

- Allows for a complete set of data for plasma modelling with speed and utility in mind
    - ➢ Structure, radiative and collisional processes

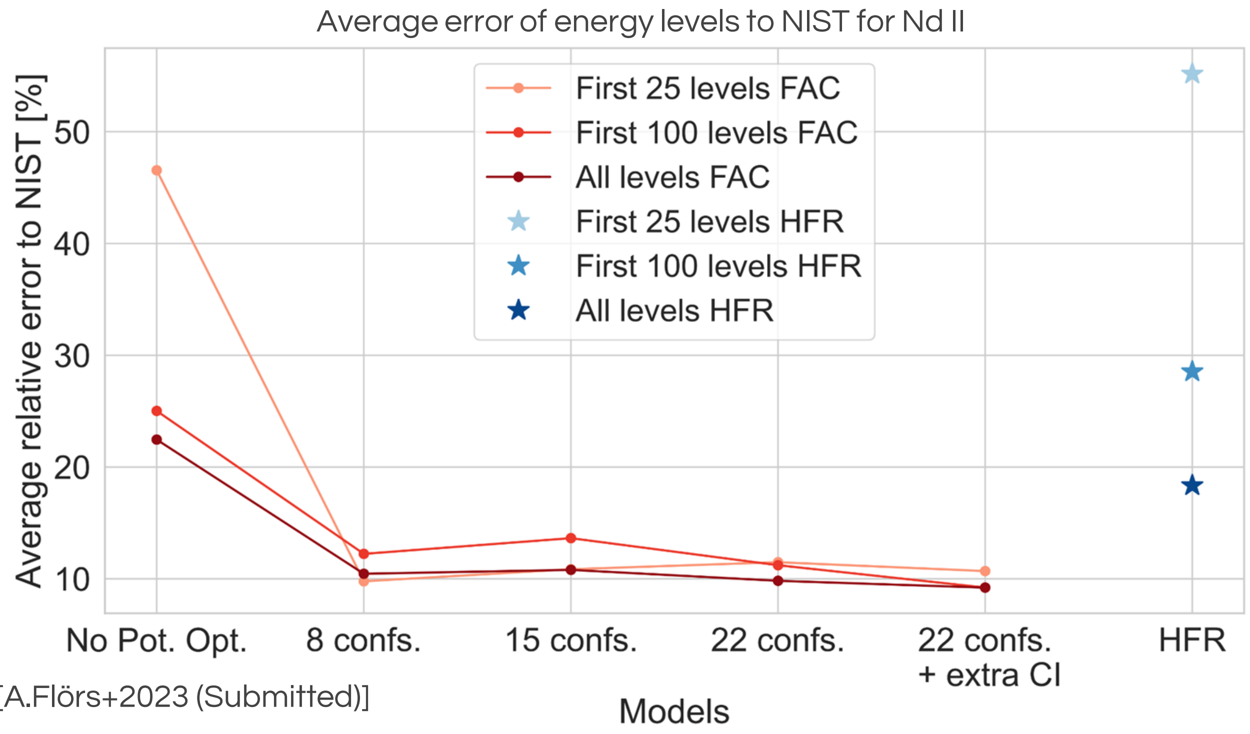
- Uses a Dirac-Fock-Slater Hamiltonian with a local central potential, computed for a fictitious mean configuration (FMC) with fractional occupation numbers

    - ➢ Orthogonality is ensured automatically → Speed increase

    - ➢ Potential not optimized for a single configuration → Accuracy issues

    - ➢ Choice of FMC is mostly arbitrary and usually constructed by hand → Major source of uncertainty

FAC – Potential Optimization



[A.Flörs+2023 (Submitted)]

- FAC correction to local potential insufficient [Lu+21, McCann+21].
- Potential optimization by changing mean configuration (weights) to minimize differences to experimental data.

FAC – Potential Optimization (Opacities)

Opacity ⇒ measure of impenetrability to radiation, given by the photons blocked because of atomic transitions.

Expansion opacity formalism

$$\kappa_{\mathrm{exp}}(\lambda) = \frac{1}{ct\rho} \sum_{l} \frac{\lambda_l}{\Delta\lambda} \underbrace{(1 - e^{-\tau_l})}_{\text{Probability of photon absorption}}$$

Probability of photon absorption

$$\tau_l = \frac{\pi e^2}{m_e c} f_l n_{i,j,k} t \lambda_l$$

Number density

Oscillator strength

Transition wavelength

FAC - Potential Optimization (Opacities)

Expansion opacity formalism

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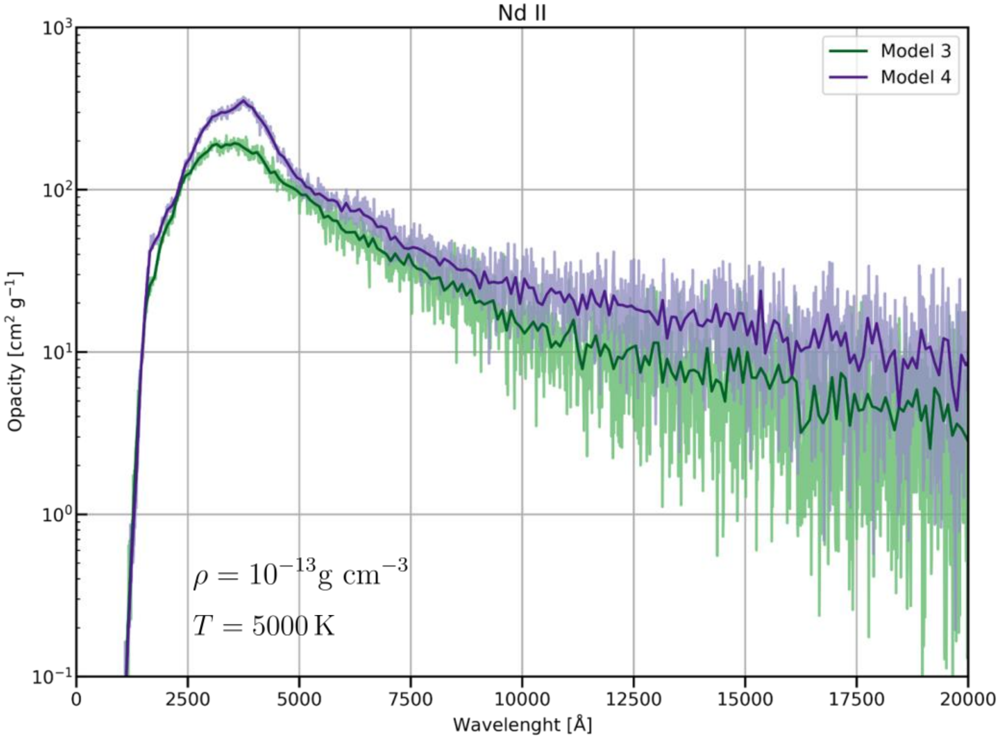
$$\tau_l = \frac{\pi e^2}{m_e c} f_l n_{i,j,k} t \lambda_l$$

- Potential optimization impacts the full spectrum.



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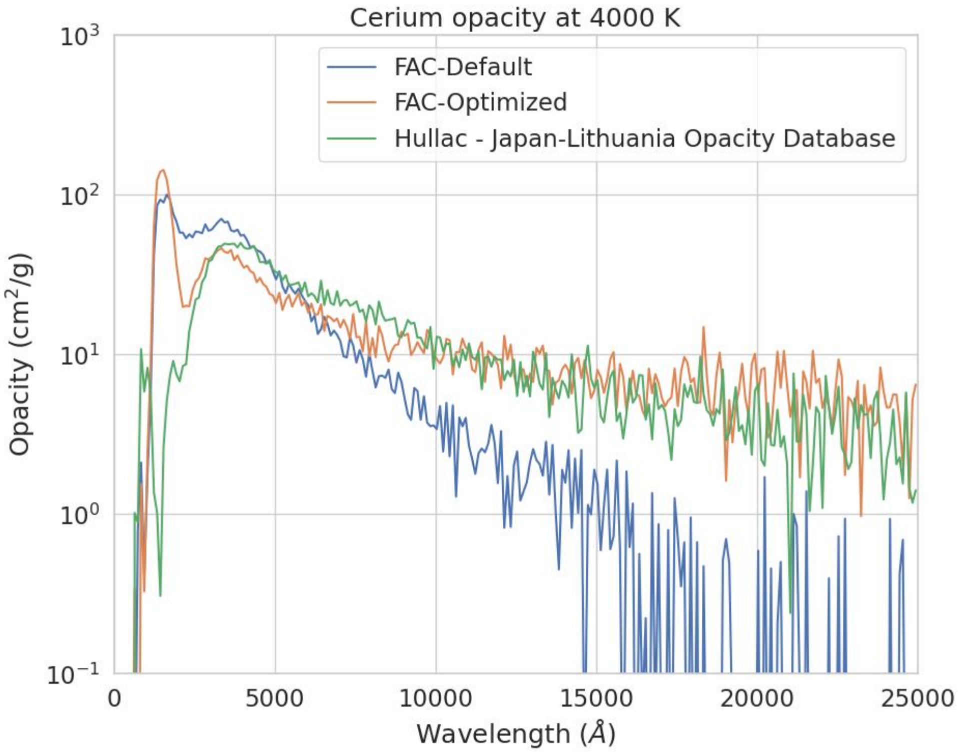
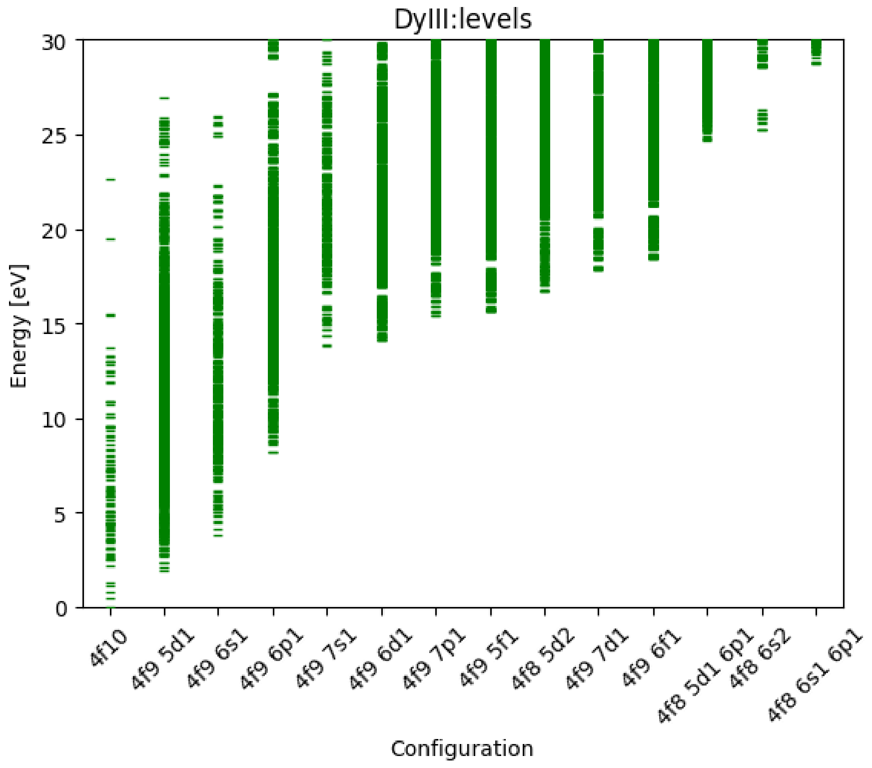
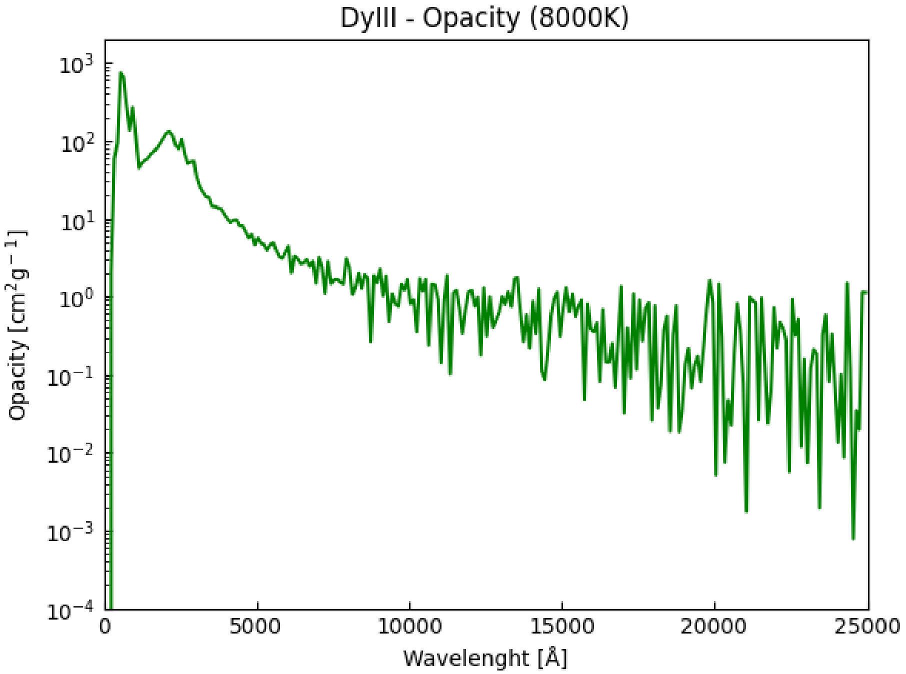
- Good general agreement with calculations with Hullac - differences at higher ionization stages.



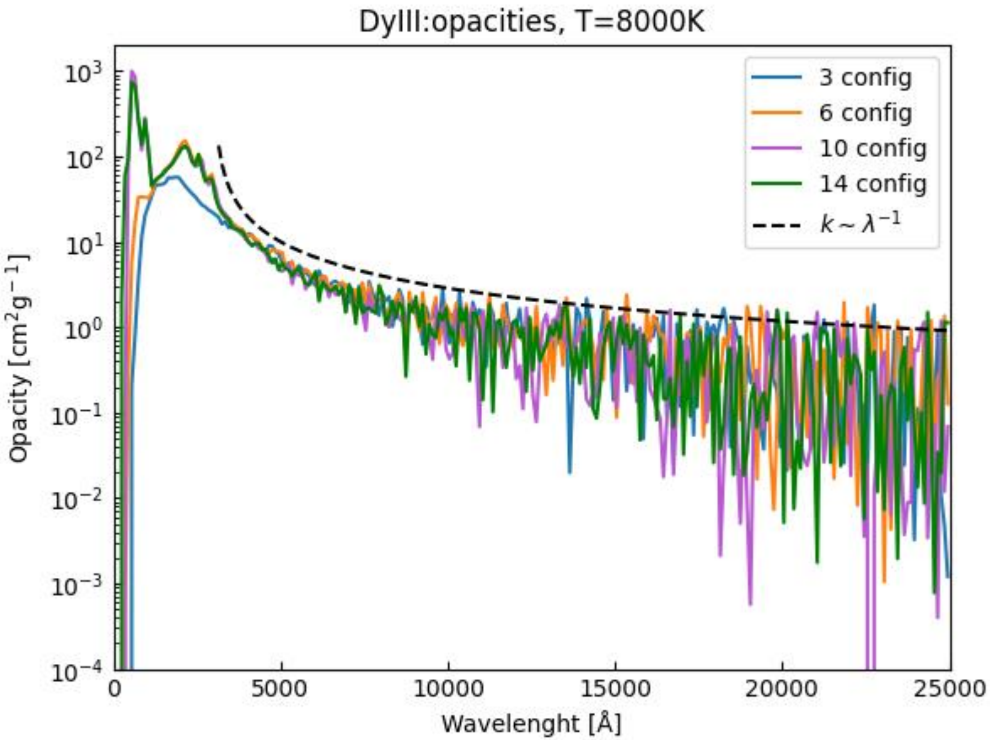
Results – Dy III



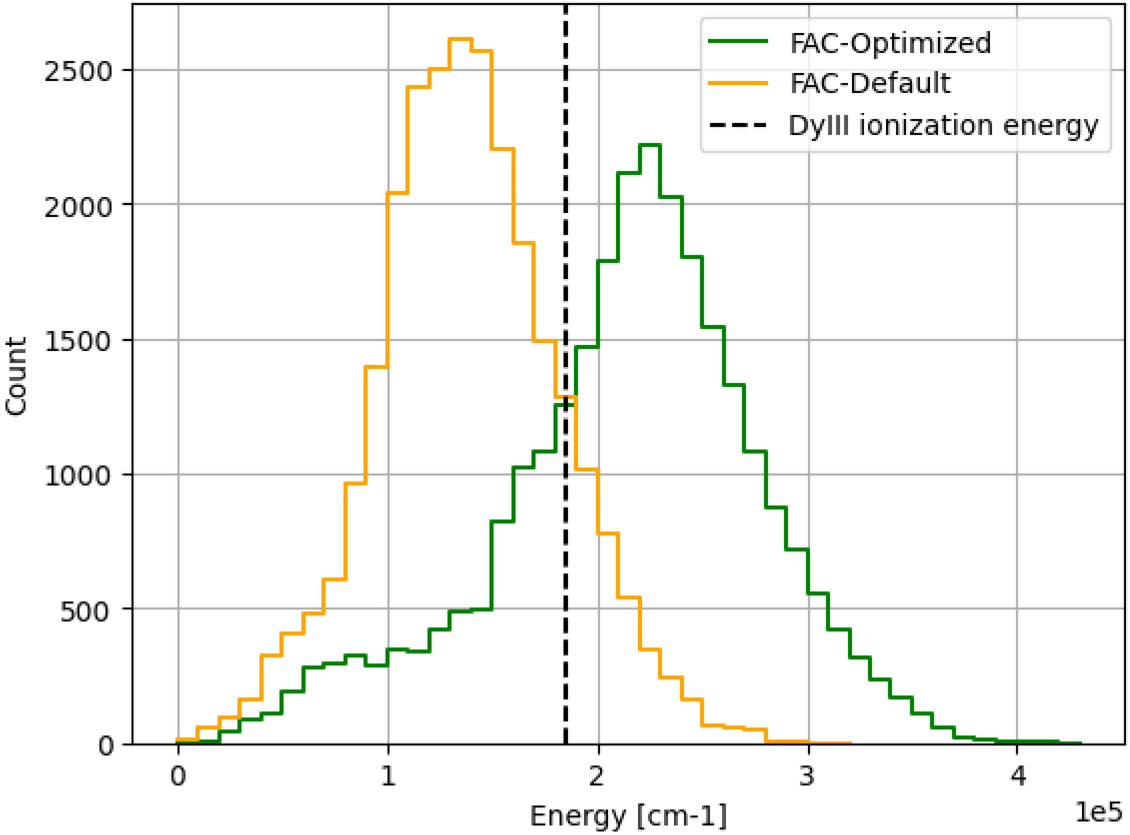


Convergence of Opacity for Dy III

- Extended set of configurations to ensure convergence
  - Higher impact at $\lambda < 5000\text{Å}$ - transitions from highly excited levels to low energy levels
  - High wavelength behaviour ruled by $\kappa \propto \lambda^{-1}$ [R.F. SIlva+ 22, G.Leck 22]



Results – Effects on level density

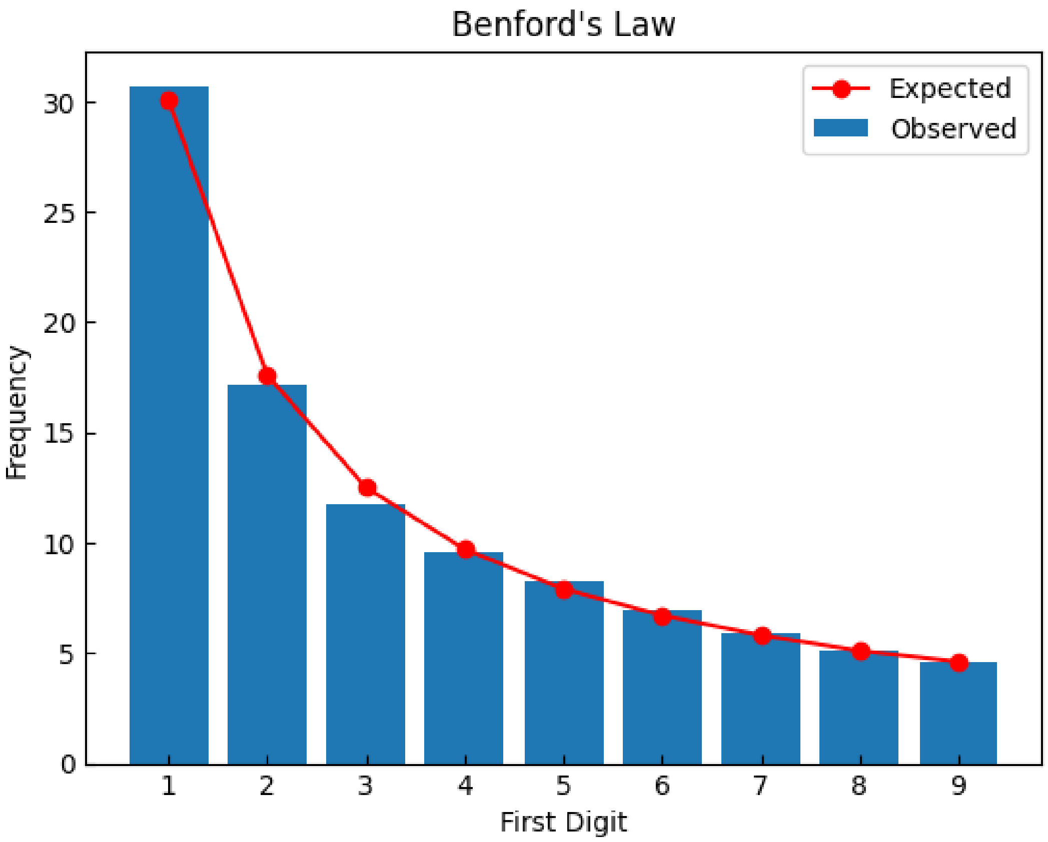


- Contrary to calibration of individual levels, optimization of the central potential impacts the full spectrum;

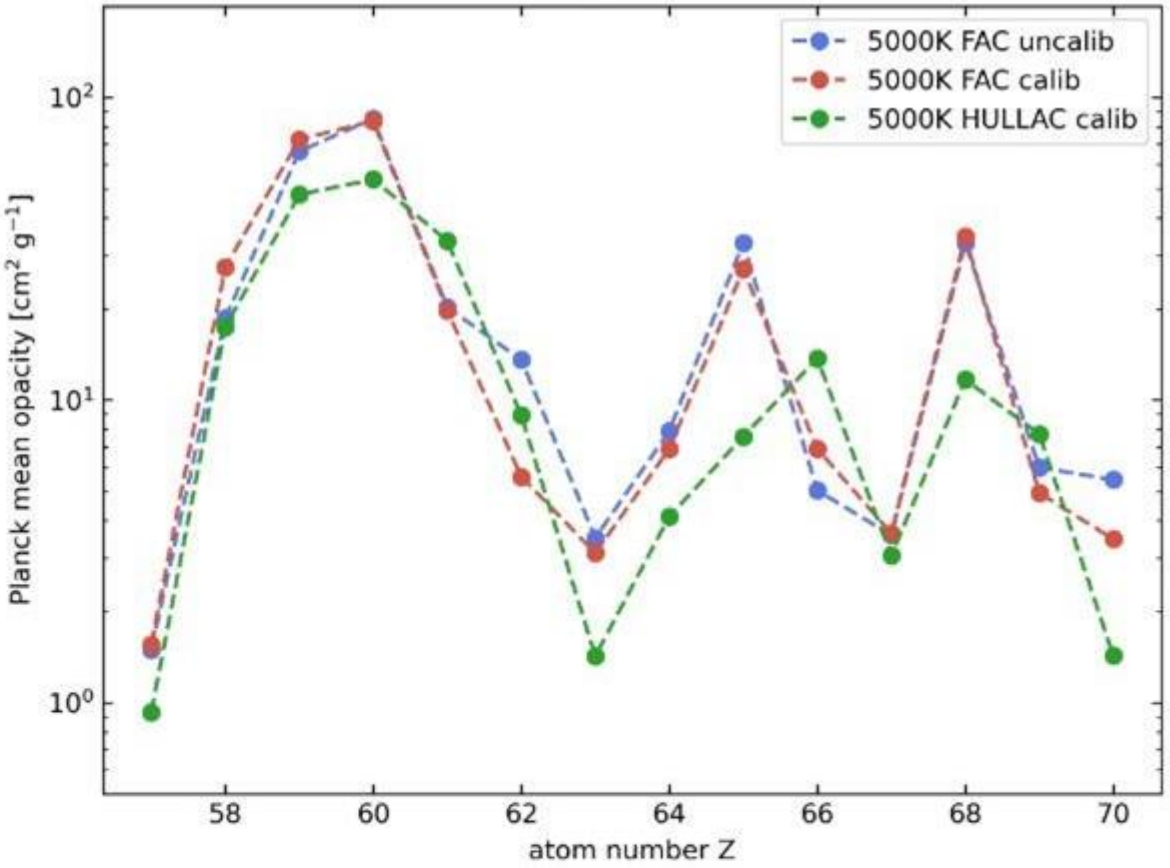
- Optimized levels typically closer to exponential behavior (up to ionization energy).

Statistical Test - CeII

- Law of anomalous numbers - leading digits distribution for sets of numerical data;
- Close match with Benford's Law, suggesting that potential optimization procedure may not be giving biased results.

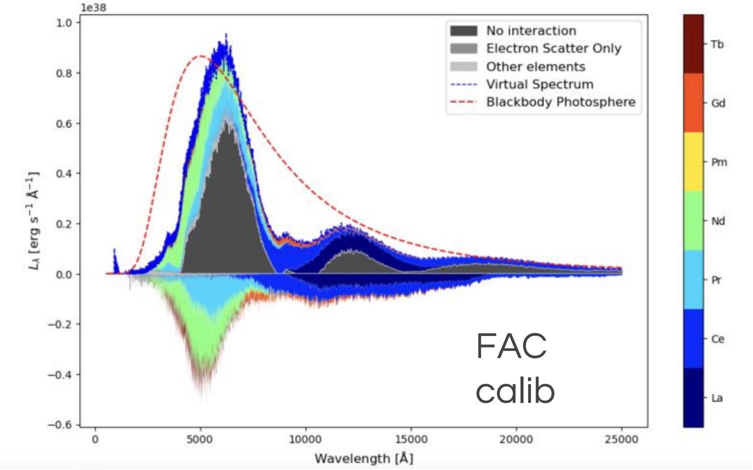


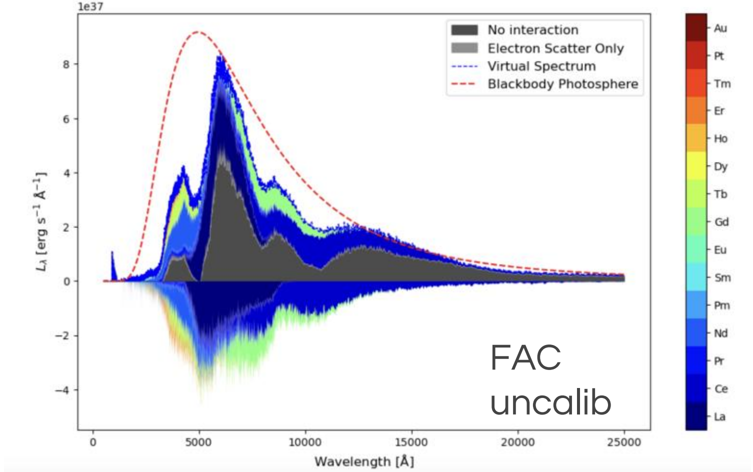
Results – Opacities



- Calibration:
  → Find the lowest energy level for each set of values with the same parity and j;
  → Shift our data to that value.

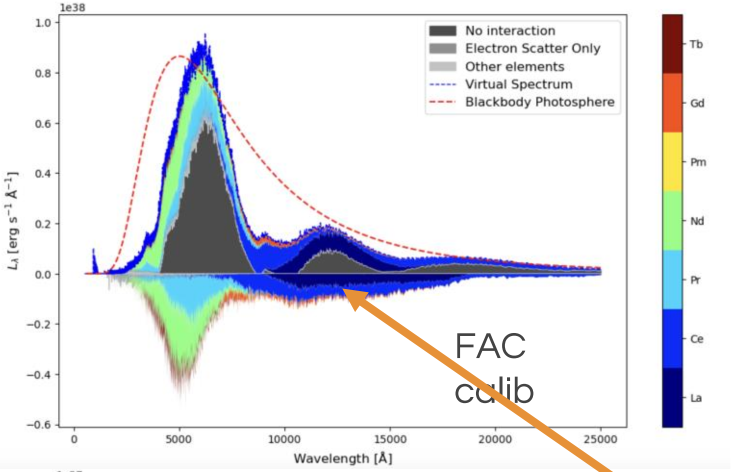
Results - Kilonova Flux

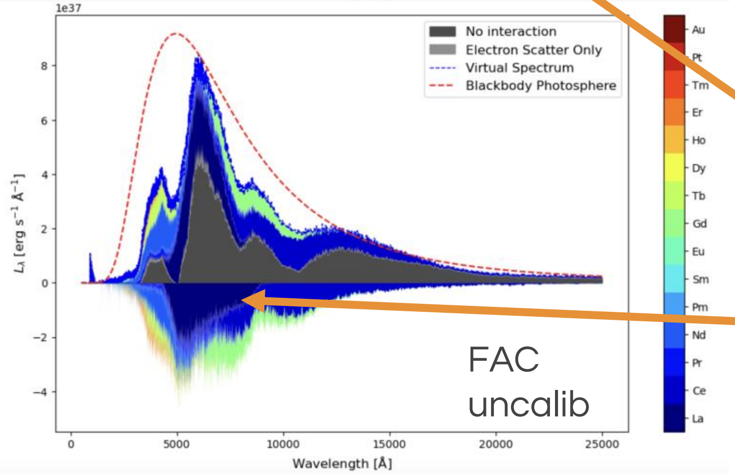




- Preliminary study into the effects of lanthanides on kilonova flux
- Too early to take conclusions about the abundance of this elements in the kilonova

Results – Kilonova Flux





- Preliminary study into the effects of lanthanides on kilonova flux
- Too early to take conclusions about the abundance of this elements in the kilonova

[Domoto+2022]

Table 3. Summary of calibrated lines for La III. We list only lines that adopt theoretical gf-values with $\lambda > 7000$ Å and $\log gf > -3$.

	λ_{vac} [a] (Å)	λ_{air} [b] (Å)	Lower level	E_{lower} [c] (cm^{-1})	Upper level	E_{upper} [d] (cm^{-1})	$\log gf$ [e]
La III	13898.270	13894.471	$5d\ ^2D_{3/2}$	0.00	$4f\ ^2F^o_{5/2}$	7195.14	−0.749
	14100.037	14096.183	$5d\ ^2D_{5/2}$	1603.23	$4f\ ^2F^o_{7/2}$	8695.41	−0.587
	17882.977	17878.094	$5d\ ^2D_{5/2}$	1603.23	$4f\ ^2F^o_{5/2}$	7195.14	−1.938

Summary and future work

- Our goal is to provide a complete set of atomic data to be used in the characterization of kilonova light curves and spectra
  - → Benchmarking of *ab-initio* for when no experimental data is available - MCDFGME, GRASP
  - → We will make our data publicly available after publication.

- Optimisation of the mean local potential leads to very good agreement with NIST data and other structure codes (e.g. GRASP)
  - → Calibration still necessary

- Radiative transfer calculations to test the impact of different atomic datasets

COLLABORATION

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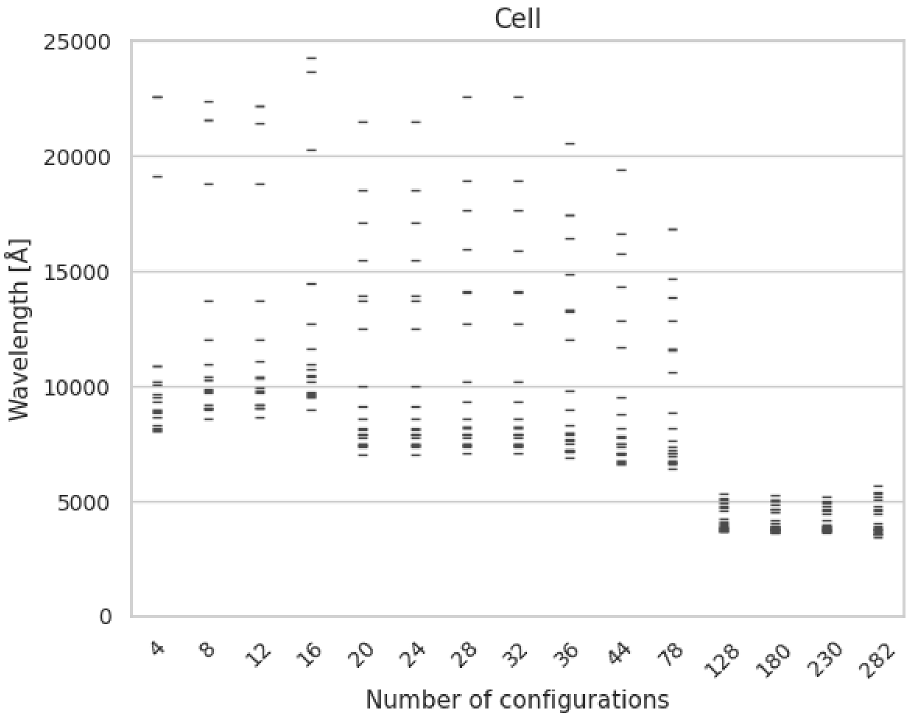
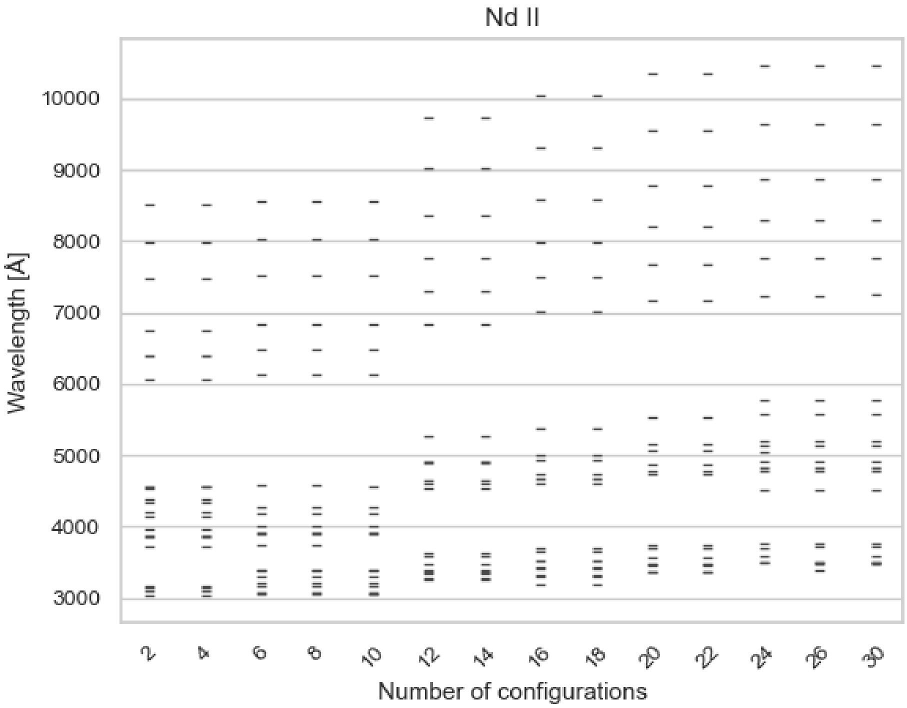
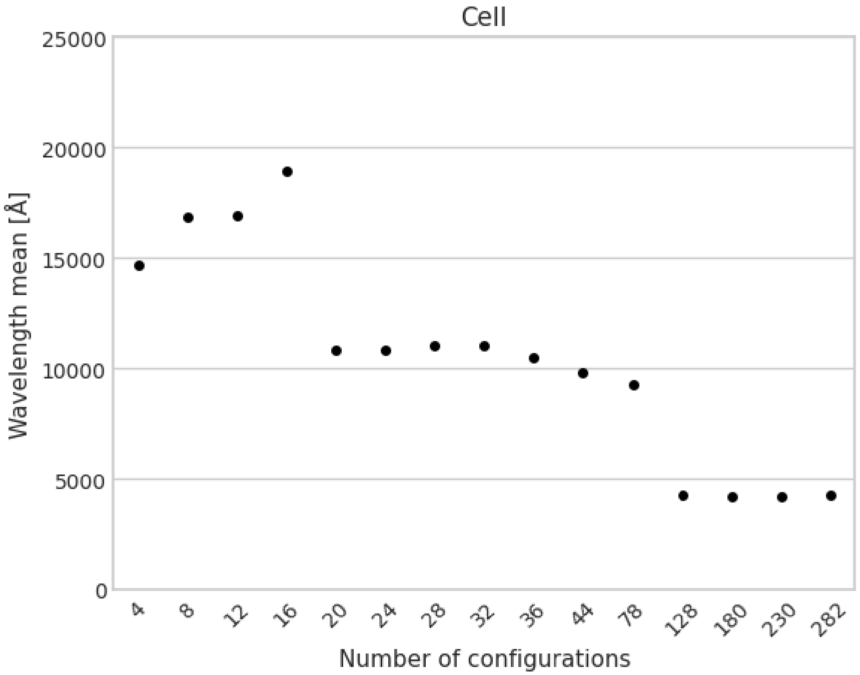
Lines Convergence

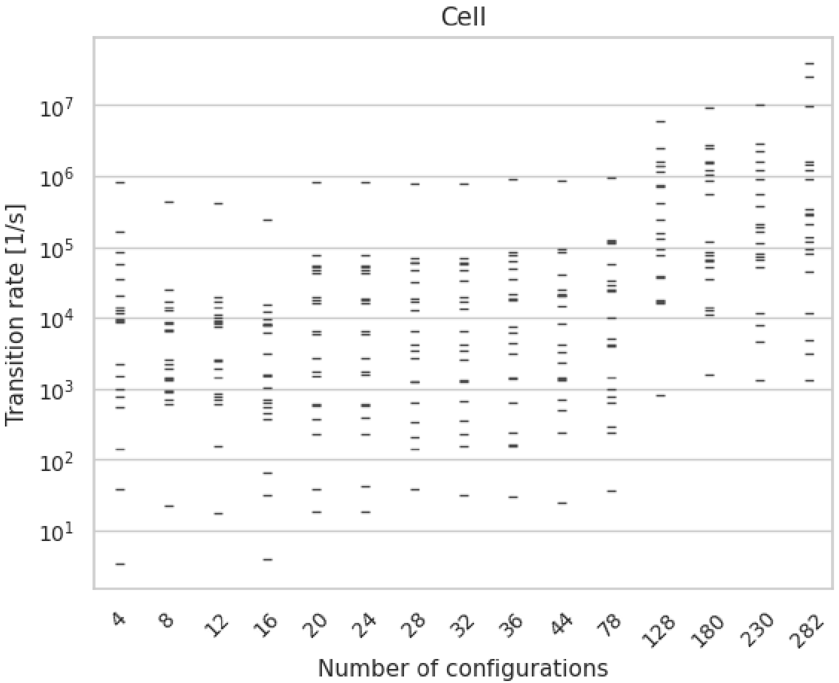




- Line convergence is achievable for simple ions;
- For complex ions (with more than 5 valence electrons) that may not be the case.

Convergence for CeII





- 20 selected transitions between 4f2 5d1 and 4f1 5d2.