Heavy Element Opacity Calculations for Kilonova Modeling

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Astrophysical Context

GW170817 event:

- Detection of gravitational waves from neutron star merger for the first time on August 17, 2017
  (Abbott B.P. et al., Phys. Rev. Lett. 119, 161101, 2017)

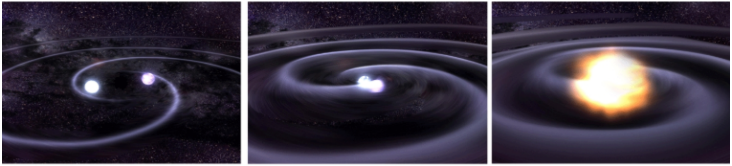
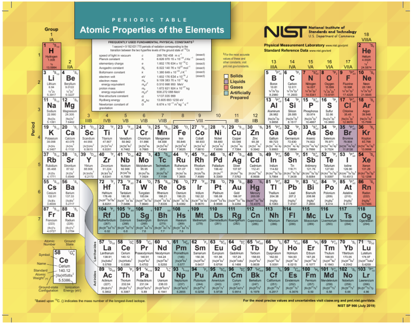


Figure 1: Evolving neutron star binary system (NASA/CXC/GSFC/T.Strohmayer)

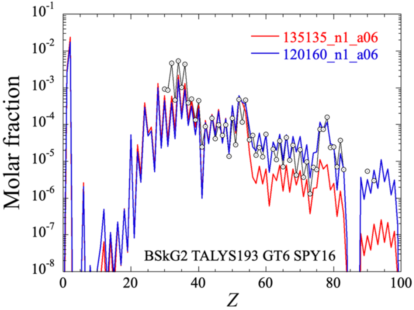
- Also produces electromagnetic signal powered by the ejection of hot and radioactive matter: kilonova (KN)

Astrophysical Context

– Heavy elements ($Z > 26$) are abundant in Kilonovae.
– Lanthanides and actinides dominate the KN opacity due to their large spectral density (open f-subshell) and abundances.



Periodic Table (NIST)



KN Abundances

(Goriely & Just, Private Communication)

Theoretical Methods: Atomic Structure

- **Multi-configurational Dirac-Hartree-Fock (GRASP2018)**:
  - Relativistic method based on the Dirac equation
  - Introduction of correlation effects in an explicit way
  - QED corrections added in a peturbative way

  valence-valence + core-valence model: allowing SD excitations from spectroscopic orbitals towards some correlation orbitals

- **Configuration interaction with MBPT corrections (AMBiT)**:
  - Relativistic method based on the Dirac equation
  - Introduction of valence correlation effects in an explicit way
  - MBPT treatment of core-core and core-valence correlation effects
  - QED corrections added in a peturbative way

Theoretical Methods: Atomic Structure

- **Pseudo-relativistic Hartree-Fock (Cowan's code)**:
  - Based on the Schrodinger equation
  - Introduction of valence correlation effects in an explicit way
  - Relativistic corrections added in a perturbative way

  Orbitals obtained for each configuration by solving the HF equations
  Codes actually developped by Cowan (1981) for opacity computation purposes

Theoretical Methods: Atomic Structure

Comparing atomic data between methods and choosing HFR results to calculate opacities

Advantage of HFR method:
$\rightarrow$ Calculation is relatively quick, even for a large number of configurations considered (large number of transitions)
$\rightarrow$ States from all the configurations are optimized

$\Rightarrow$ Suitable to compute physical quantities as opacity which requires to consider large numbers of transitions

Some examples:
La VII: 818 233 lines
Ce VIII: 1 113 548 lines
Sm V: 17 267 783 lines
Sm VIII: 30 795 559 lines

Theoretical Methods: Expansion Opacity

Use of **expansion formalism for bound-bound opacities**:

$$\kappa_{\text{exp}}^{\text{bb}}(\lambda) = \frac{1}{\rho c t} \sum_{l} \frac{\lambda_l}{\Delta\lambda}(1 - e^{-\tau_l}) \tag{1}$$

with Sobolev optical depth:

$$\tau_l = \frac{\pi e^2}{m_e c} t n_l \lambda_l f_l \tag{2}$$

Radiative wavelength λ_l and oscillator strength f_l are needed to compute the expansion opacity (+ level population n_l)

Theoretical Methods: Expansion Opacity

Using Boltzmann:

$$n_l = \frac{n}{U_j(T)} g_l e^{-E_l/k_B T} \tag{3}$$

where:

$$n = \frac{\rho}{A m_p} X_j \quad \text{(Banerjee et al. (2020))} \tag{4}$$

and Saha:

$$X_j = \frac{n_j}{\sum_j n_j} \tag{5}$$

$$\frac{n_j}{n_{j-1}} = \frac{\pi m_e k_B T \, U_j(T)}{h^2 n_e U_{j-1}(T)} e^{-\chi_{j-1}/k_B T} \tag{6}$$

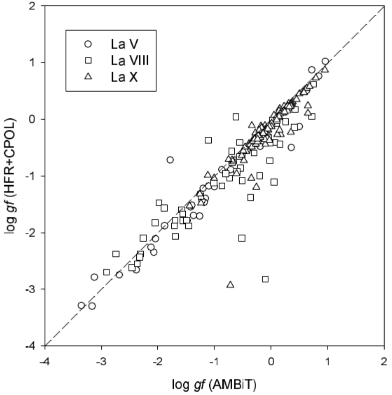
Previous Studies

Recent studies exist for KN opacities, *e.g.*:

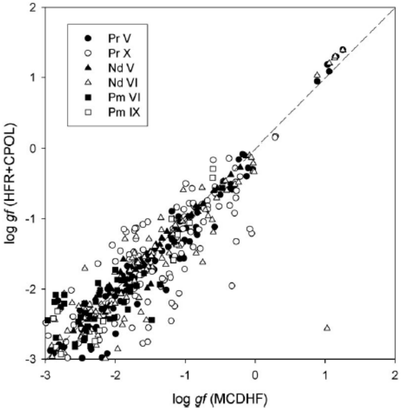
- Gaigalas *et al.*, ApJS, **240**, 29 (2019): Nd II–IV with MCDHF
- Fontes *et al.*, MNRAS, **493**, 4143 (2020): All lanthanides I–IV using Los Alamos codes
- Tanaka *et al.*, MNRAS, **496**, 2 (2020): Fe to Ra I–IV with HULLAC
- Flörs *et al.*, MNRAS, accepted (2023): Nd & U II–III with FAC and HFR
- Fontes *et al.*, MNRAS, **519**, 2862 (2023): Ac to No I–IV using Los Alamos codes
- Banerjee *et al.*, A& A, **934**, 2 (2022): Nd, Sm, Eu I–XI with HULLAC
- Banerjee *et al.*, arXiv:2304.05810 [astro-ph.HE] (2023): La to Ra V–XI with HULLAC

⇒ Few works on actinides and moderately-charged ions!

Comparisons of Oscillator Strengths



Carvajal Gallego *et al.* 2022

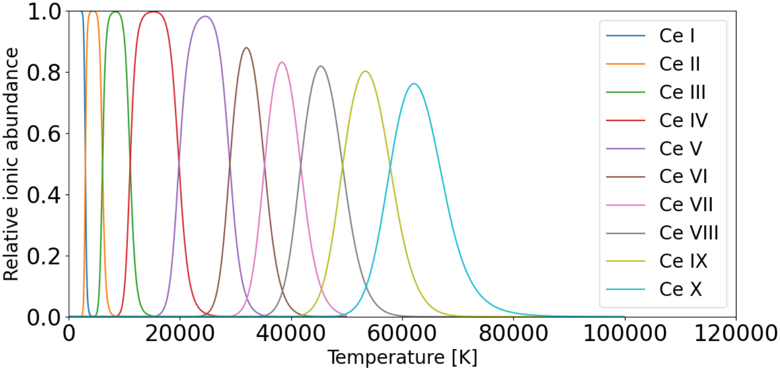


Carvajal Gallego *et al.* 2023

Early-Phase Kilonovae: Physical Conditions

Early-phase kilonovae
$\rightarrow t = 0.1\ d$; $\rho = 10^{-10} g\ cm^{-3}$ and $20000\ K < \mathrm{T} < 50000\ K$ (Combi & Siegel, 2023)
$\rightarrow$ moderately-charged lanthanide ions

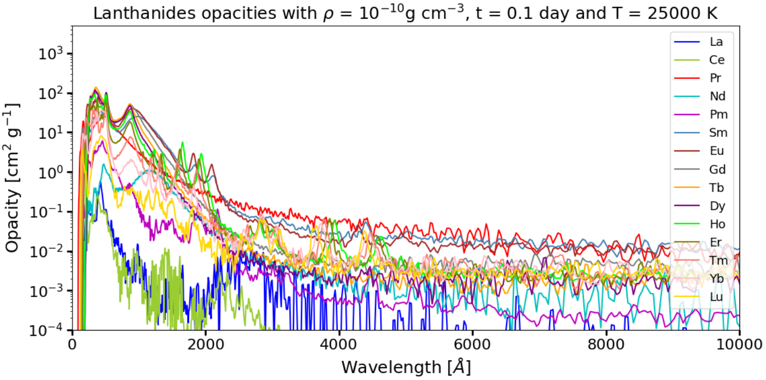
Ce ions V - VII: $25000\ \mathrm{K} < \mathrm{T} < 40000\mathrm{K}$



Early-Phase Kilonovae: Lanthanide Opacities

Tb and Dy are predominant in UV and Sm and Pr have the larger opacity in IR

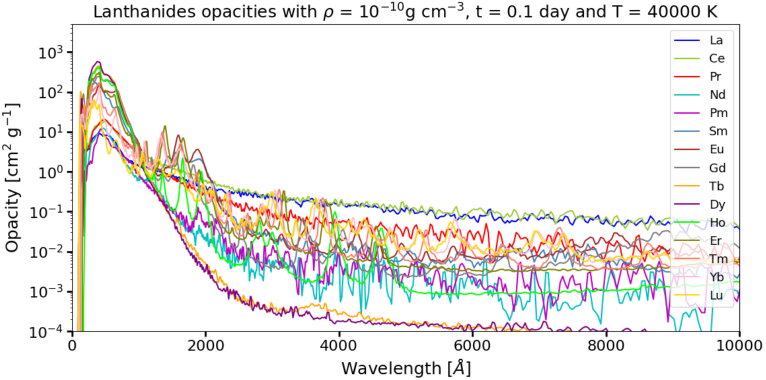
La and Ce have the smallest opacity in all the wavelength range



Carvajal Gallego H., et al. submitted to A&A (2023)

Early-Phase Kilonovae: Lanthanide Opacities

Tb and Dy are predominant in UV while it decrease sharply in visible/IR
La and Ce have the highest opacity from visible to IR



Carvajal Gallego H., et al. submitted to A&A (2023)

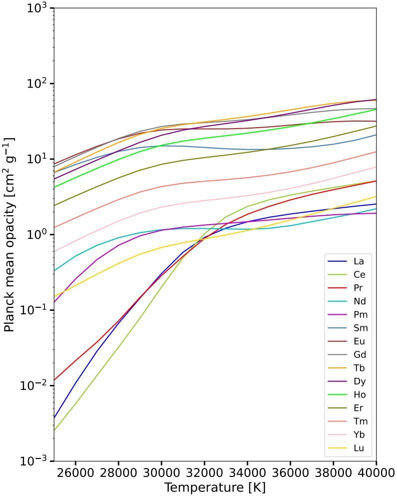
Planck mean opacities defined as

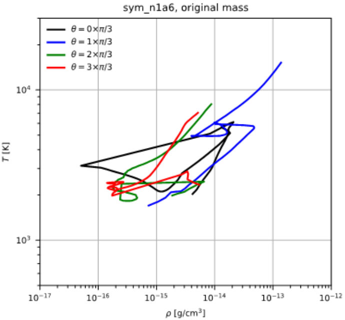
$$\kappa_P = \frac{\int \kappa_\lambda B_\lambda(T)d\lambda}{\int B_\lambda(T)d\lambda} \qquad (7)$$

Computed for all lanthanide ions from V - VII

→ At T = 25 000 K: Eu has the largest opacity

→ At T = 40 000 K: Dy has the largest opacity





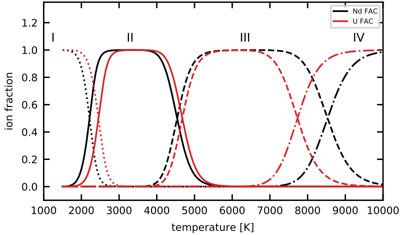
Temperature VS density of the KN photosphere

O. Just and S. Goriely, private communication

$\Rightarrow 10^{-17}$ g/cm$^3 < \rho < 10^{-13}$ g/cm^3

and

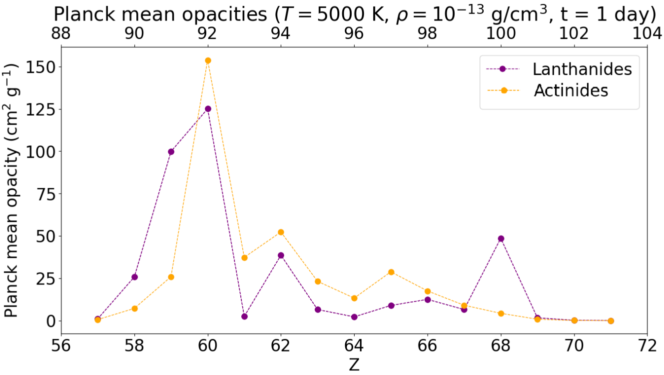
$1000 \text{ K} < T < 10000 \text{ K}$



Flörs, Silva, Deprince *et al.* 2023 (accepted)

$\Rightarrow$ Only the first ionization stages (I – IV) of the elements are present in the KN ejecta 1 day after the NSM

Lanthanide & Actinide Planck Mean Opacities



Deprince *et al.* in preparation (2023)

⇒ Opacity for U ($Z = 92$) as large as Nd ($Z = 60$) or even greater

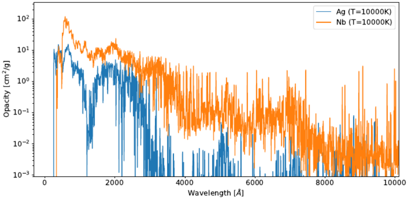
⇒ Actinides as important as lanthanides

4d-Transition Element Opacities

$$\rho = 10^{-13} \text{ g/cm}^3, \text{ t} = 1 \text{ day}$$

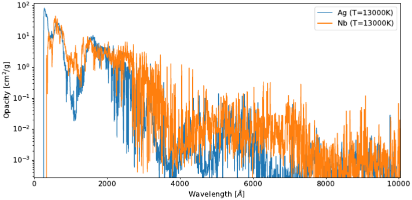
T = 10000 K

Ag (blue); Nb (orange)



T = 13000 K

Ag (blue); Nb (orange)

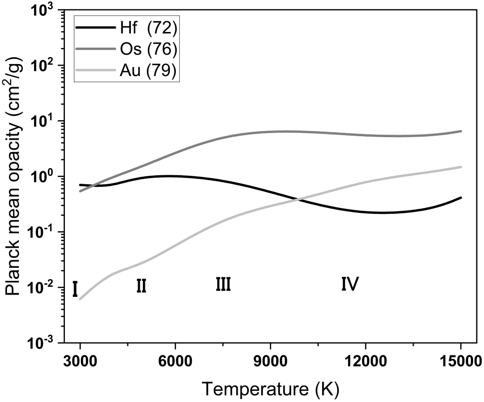


Ben Nasr *et al.* submitted to A&A (2023)

⇒ At T=10000 K Nb dominates over Ag
but at T=13000 K Ag starts to equate Nb

5d-Transition Element Planck Mean Opacities

$$\rho = 10^{-13}\ \text{g/cm}^3,\ t = 1\ \text{day}$$



Ben Nasr *et al.* in preparation (2023)

⇒ At T=3000 K Hf dominates, but for higher T it is Os that remains dominant. At T=10000 K, Au surpasses Hf.

Conclusion & Prospects

CONCLUSION

– Atomic data and opacities for early-phase KN:
⇒ All moderately-charged (V – VII) lanthanides done!

– Atomic data and opacities for 1-day post merger KN:
⇒ All lowly-charged (I – IV) lanthanides and actinides done!
⇒ Some lowly-charged (I – IV) 4d-(Nb,Ag) and 5d-(Hf,Os,Au) elements done!

PROSPECTS

– Computation of atomic data and opacities for all the missing elements from Ca to Ra for charge states I – IV using HFR.

– HFR method has limits: compute opacities for lanthanide ions VIII - X
⇒ investigation of a statistical approach

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Thank you for your attention!

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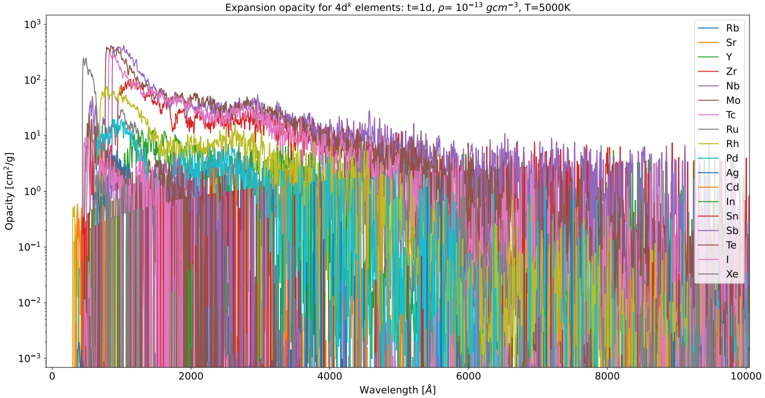
Row 5 Element Opacities ($Z = 37 - 54$)

$$\rho = 10^{-13}\ \text{g/cm}^3,\ \text{t} = 1\ \text{day},\ \text{T} = 5000\ \text{K}$$



Preliminary results!