Atomic calculations of forbidden lanthanide transitions for modeling nebular-phase kilonova spectra

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In March 2023, astrophysicists detected a gamma ray burst associated with what could be a merger of compact objects followed by a transient afterglow. After analyzing the spectra, they found some similarity with the AT2017gfo kilonova spectra suggesting the presence of such phenomena. The particularity with this kilonova event is that the spectrum has been recorded at late time after the merger [1]. At these times, the kilonova is said to be in his nebular phase. Conditions are such that the temperature is really low and the ionization stage does not exceed the doubly charged species. Only low-lying levels, such as metastable levels, are populated giving rise to so-called emission forbidden lines, such as the magnetic dipole (M1) and electric quadrupole (E2) transitions. Element identification in nebular phase spectra is quite challenging since atomic data and especially forbidden line lists for heavy elements are scarce in the literature. In this work, atomic calculations of M1 and E2 transition probabilities between low-lying levels in doubly and singly ionized lanthanides were performed using the fully-relativistic Multi-Configurational-Dirac-Hartree-Fock (MCDHF) and pseudo–relativistic Hartree-Fock (HFR) method.

AT2023vfi kilonova

- Second spectroscopic observation of a kilonova
- Observation of emission features around 2.1 µm and 4.4 µm
  - Possible presence of forbidden transitions from heavy r-process elements in the kilonova spectra at late times

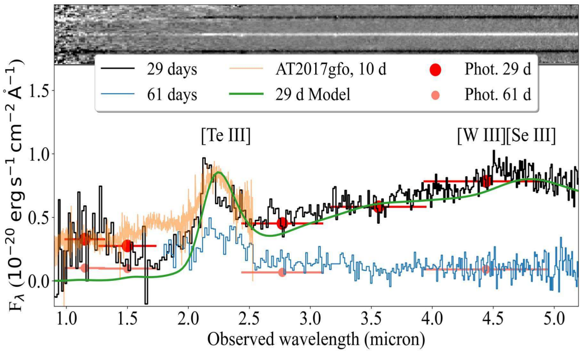

Fig 1 *JWST/NIRSpec spectra of the AT2023vfi kilonova at 29 and 61 days after the event [1]*

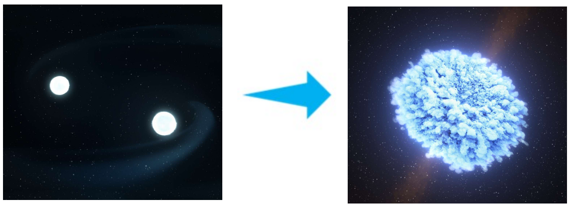

Fig 2 Artistic view of a compact object merger followed by a transient afterglow called kilonova)

Theoretical methods

Multiconfiguration Dirac-Hartree-Fock

- Based on the Dirac-Coulomb equation [2]
- Multiconfiguration approach
- QED corrections + Breit transverse interaction correction
- GRASP package [3]

Pseudo–relativistic Hartree-Fock

- Based on the Schrödinger equation [4]
- Multiconfiguration approach
- One-body relativistic corrections (spin-orbit, mass-velocity, Darwin)
- Semi-empirical calculations with adjustment of radial parameters

[1] A. Levan, et al., *Nature* **626**, 737-741 (2024).
[2] I. P. Grant, *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation* (Springer, New York, 2007).
[3] C. Froese Fischer, et al., *Comput. Phys. Commun.* **237**, 184 (2019).
[4] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[5] J. H. Gillanders, S. J. Smartt, *MNRAS* **538**, 1663-1689 (2025).

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M1 and E2 transition probabilities

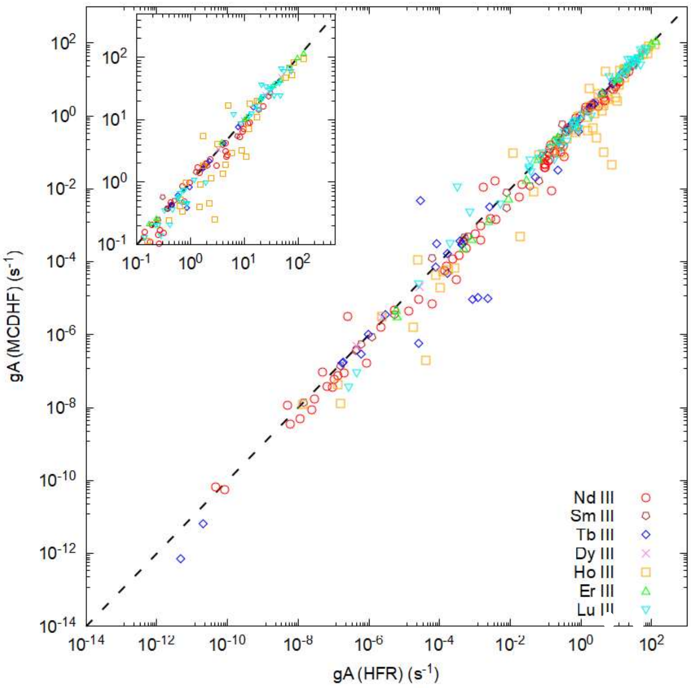

Fig 3 *Transition probabilities comparison between HFR and MCDHF for Nd-Sm-Tb-Dy-Ho-Er III and Lu II*

Astrophysical applications

- More than 1000 lines with experimentally known levels computed

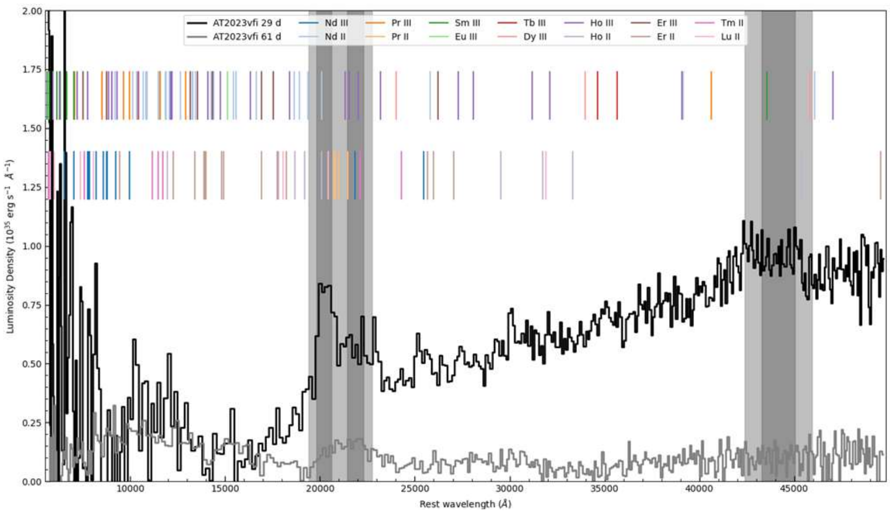

Fig 4 *Most intense forbidden transitions ($gA > 10^{-1}\ s^{-1}$) overplotted on the +29 d and +61 d JWST spectra of AT2023vfi (rest frame) [1][5] . Colored vertical lines mark the transition wavelengths. Shaded regions correspond to ±0.02c and ±0.04c velocity intervals around selected features.*

- Strong forbidden transitions and possible candidates :
  - 3 [Ho III], 1 [Ho II], 1 [Nd III], 1 [Nd II], 5 [Pr II], 1 [Tm II] and 1 [Lu II] around 2.1 µm
  - 1 [Dy III], 1 [Sm III] and 1 [Ho II] around 4.4 µm

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