Multiplatform computations of M1 and E2 transition probabilities in lanthanide ions for kilonova nebular-phase analysis

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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 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 peaks around 2.1 µm and 4.4 µm
  - Possible presence of forbidden transitions from heavy r-process elements in the kilonova spectra at late time epoch

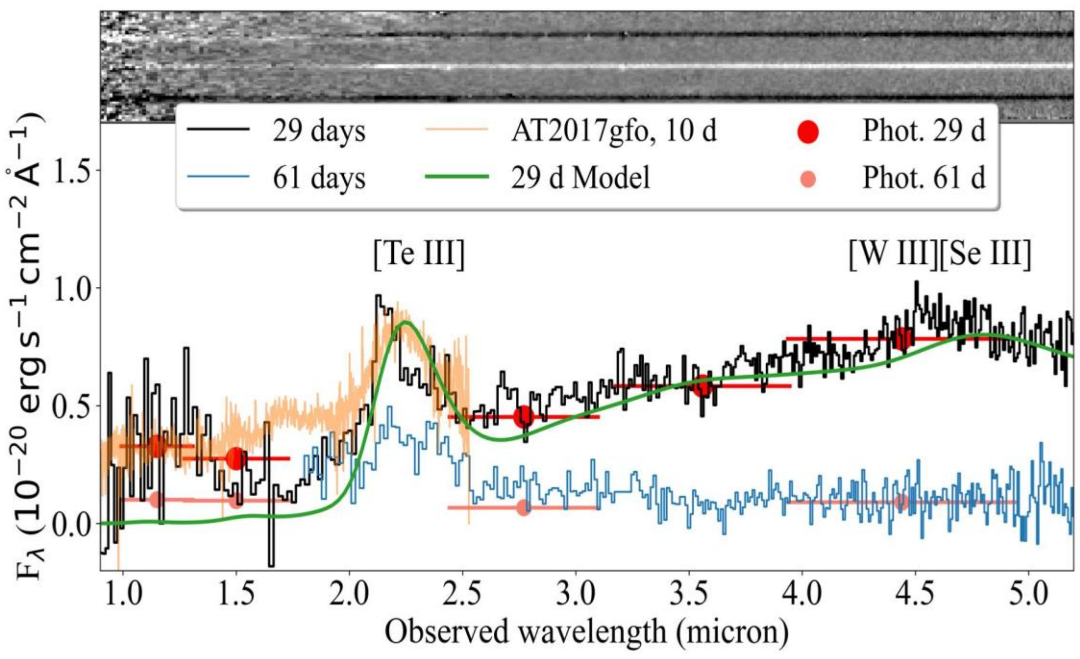

Fig 1 JWST/NIRSpec spectra of the AT2023vfi kilonova at 29 and 61 days after the event [1]

Fig 2 Artistic view of a compact object merger followed by a transient afterglow called kilonova (www.svs.gsfc.nasa.gov/12740)

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 calculation 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, New York: Springer (2007).
[3] C. Froese Fischer, *et al.*, Comput. Phys. Commun. 237, 184 (2019).
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[6] M. Ding , *et al.*, A&A 684, A149 (2024).
[7] J.-F. Wyart, *et al.*, Physica Scripta 56(5), 446 (1997).
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M1 and E2 transition probabilities

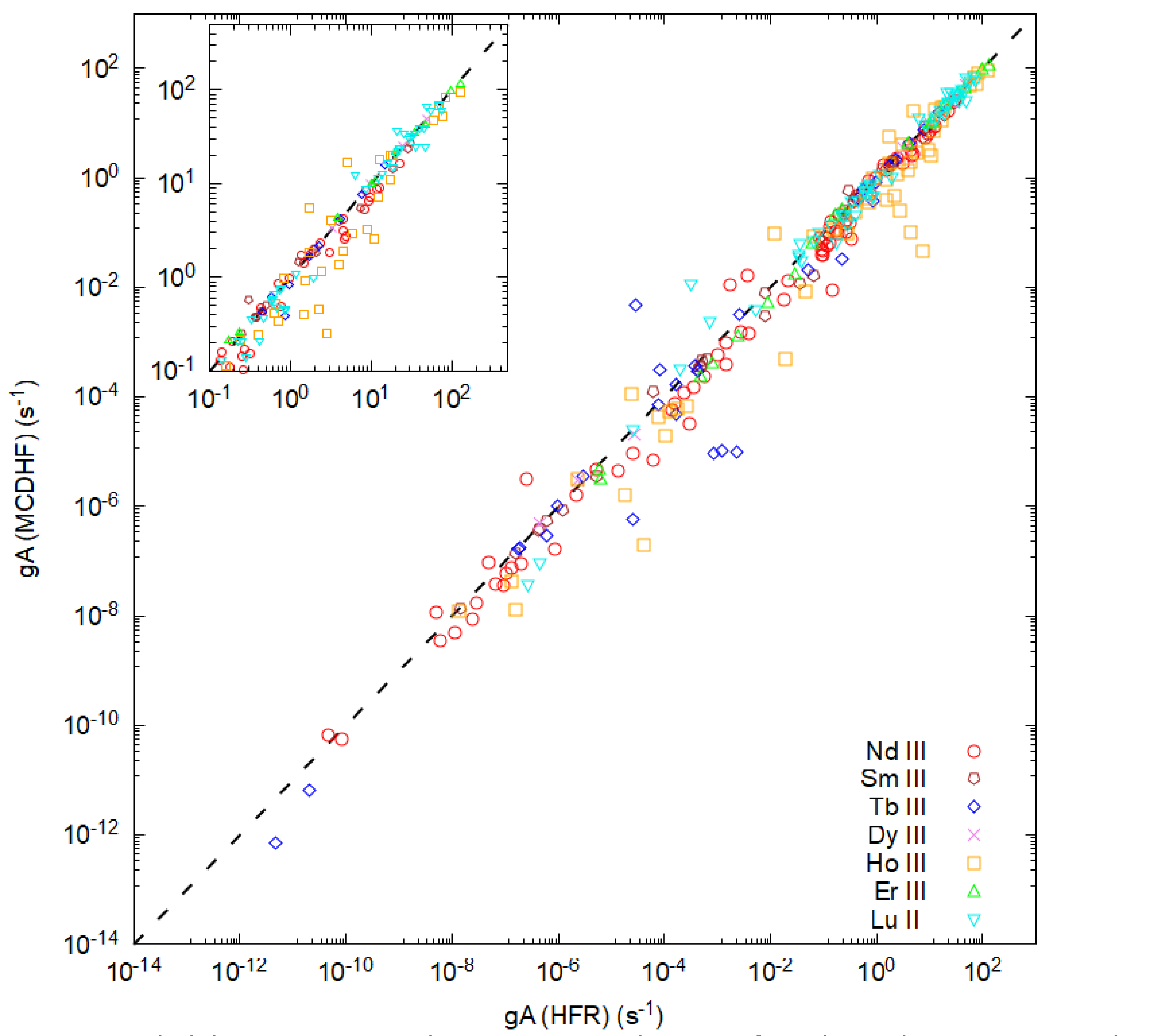

Fig 3 Transition probabilities comparison between HFR and MCDHF for Nd-Sm-Tb-Dy-Ho-Er III and Lu II

Astrophysical applications

- 482 lines with experimentally known levels [5-8]

Species	Transition Type	Lower level			Upper Level			λ_{exp} (Å)	gA_{HFR} (s^{-1})
		Conf.	Term	E (cm^{-1})	Conf.	Term	E (cm^{-1})		
Sm III	M1	$4f^6$	$^7F_2$	814	$4f^6$	$^5D_1$	15870	6641	1.87E+01
Nd III	M1	$4f^4$	$^5I_5$	1138	$4f^4$	$^3K_6$	14064	7736	9.20E+00
Ho III	M1	$4f^{11}$	$^4I_{11/2}°$	8645	$4f^{11}$	$*_{9/2}°$	21534	7758	5.88E+01
Nd III	M1	$4f^4$	$^5I_6$	2388	$4f^4$	$^3K_7$	15154	7833	1.27E+01
Ho III	M1	$4f^{11}$	$^4I_{13/2}°$	5439	$4f^{11}$	$^2H2_{11/2}°$	16891	8732	1.26E+02
Nd III	M1	$4f^4$	$^5I_7$	3715	$4f^4$	$^3K_7$	15154	8742	1.19E+01
Er III	M1	$4f^{12}$	$^3H_5$	6970	$4f^{12}$	$^1G_4$	18384	8761	1.30E+02
Nd III	M1	$4f^4$	$^5I_8$	5093	$4f^4$	$^3K_8$	16459	8798	2.26E+01
Pr III	M1	$4f^3$	$^4I_{11/2}°$	1398	$4f^3$	$^2H2_{11/2}°$	12495	9012	2.36E+00
Pr III	M1	$4f^3$	$^4I_{9/2}°$	0	$4f^3$	$^2H2_{9/2}°$	10033	9967	5.71E+00
Pr III	M1	$4f^3$	$^4I_{13/2}°$	2893	$4f^3$	$^2H2_{11/2}°$	12495	10415	5.51E+00
Pr III	M1	$4f^3$	$^4I_{11/2}°$	1398	$4f^3$	$^2H2_{9/2}°$	10033	11581	3.71E+00
Ho III	M1	$4f^{11}$	$^4F_{9/2}°$	13329	$4f^{11}$	$*_{9/2}°$	21534	12189	6.87E+01
Er III	M1	$4f^{12}$	$^3H_4$	10786	$4f^{12}$	$^1H_4$	18384	13161	3.43E+01
Er III	M1	$4f^{12}$	$^3F_4$	5082	$4f^{12}$	$^3F_3$	12473	13530	4.63E+01
Er III	M1	$4f^{12}$	$^3H_6$	0	$4f^{12}$	$^3H_5$	6970	14348	9.89E+01
Er III	M1	$4f^{12}$	$^3F_4$	5081	$4f^{12}$	$^3H_4$	10785	17532	2.01E+01
Lu II	M1	5d6s	$^3D_1$	11796	5d6s	$^1D_2$	17333	18062	1.17E+00
Ho III	M1	$4f^{11}$	$^4I_{15/2}°$	0	$4f^{11}$	$^4I_{13/2}°$	5439	18387	8.25E+01
Lu II	M1	5d6s	$^3D_2$	12435	5d6s	$^1D_2$	17333	20419	1.38E-01
Nd III	M1	$4f^4$	$^5F_2$	10774	$4f^4$	$^5G_3$	15350	21855	3.18E-01
Ho III	M1	$4f^{11}$	$^4F_{9/2}°$	13329	$4f^{11}$	$^4F_{17/2}°$	17868	22031	1.72E+01
Dy III	M1	$4f^{10}$	$^5I_8$	0	$4f^{10}$	$^5I_7$	4161	24031	4.83E+01
Tb III	M1	$4f^9$	$^6H_{13/2}$	2805	$4f^9$	$^6F_{11/2}$	6470	27282	8.62E-01
Ho III	M1	$4f^{11}$	$^4I_{13/2}°$	5439	$4f^{11}$	$^4I_{11/2}°$	8645	31191	1.89E+01
Dy III	M1	$4f^{10}$	$^5I_7$	4161	$4f^{10}$	$^5I_6$	7103	33992	2.47E+01
Tb III	M1	$4f^9$	$^6H_{15/2}$	0	$4f^9$	$^6H_{13/2}$	2805	35655	1.48E+01
Pr III	M1	$4f^3$	$^2H2_{9/2}°$	10033	$4f^3$	$^2H2_{11/2}°$	12495	40622	1.63E+00
Sm III	M1	$4f^6$	$^5D_2$	17814	$4f^6$	$^5D_3$	20110	43563	3.93E+00
Dy III	M1	$4f^{10}$	$^5I_6$	7103	$4f^{10}$	$^5I_5$	9285	45828	9.85E+00
Tb III	M1	$4f^9$	$^6H_{13/2}$	2805	$4f^9$	$^6H_{11/2}$	4734	51817	7.71E+00

Table 1 Most intense forbidden transitions in the observation range of the NIRSpec onboard the JWST

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

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