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Comprehensive Atomic Data for Kilonova Spectral Modeling Beyond the Photospheric Phase

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The limited but growing set of kilonova observations following neutron star mergers has established these events as significant sites for r-process nucleosynthesis [1,2]. Despite recent advances in spectral identification of several elements in merger ejecta [see for e.g. 3], precise abundance determinations remain challenging, particularly at later evolutionary phases where non-local thermodynamic equilibrium (non-LTE) effects become dominant [4-6]. Our work addresses this challenge through expanded atomic calculations for lanthanide and actinide species, with special attention to processes critical in the low-density environments of expanding ejecta.

We utilize both the Flexible Atomic Code [7] and AUTOSTRUCTURE [8], enhancing atomic structure accuracy through our sequential model-based optimization methodology [9,10]. For selected lanthanides, actinides, and key elements identified in early kilonova spectra, we develop comprehensive datasets that include forbidden transitions and electron impact excitation often omitted in current models. Our analysis demonstrates how synthetic spectra are significantly affected when these transitions are neglected or when atomic processes are approximated using simplified formulae. This can lead to misidentification of spectral features, highlighting the importance of comprehensive atomic datasets for reliable kilonova modeling.

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[2] Levan et al. Nature 626, 737–741 (2024)
[3] Gillanders et al. MNRAS 529, 2918–2945 (2024)
[4] Gillanders et al. MNRAS stac1258 (2022)
[5] Vieira et al. Astrophys. J. 962, 33 (2024)
[6] Pognan et al. MNRAS 510, 3806 (2022)
[7] Gu et al. Can. J. Phys. 86, 675 (2008)
[8] Badnell Astrophys. Source Code Libr. ascl:1612.014 (2016)
[9] Flörs et al. MNRAS 524, 3083 (2023)
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