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Improving opacity predictions through optimization of atomic data calculations

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The 2017 observation of the electromagnetic counterpart to the gravitational wave signal GW170817 provided direct evidence that r-process elements are created in neutron-star mergers. The electromagnetic transient, also known as a kilonova, has revealed two distinct ejecta components: one containing heavy r-process material, including lanthanides and potentially actinides, and a second one characterized by low lanthanide abundance [1]. Spectroscopic data can often be used to identify features due to specific elements (e.g., Sr II [2]). However, having accurate atomic data is crucial for the interpretation of observed spectra, as even small relative errors (e.g., a few percent) in the transition wavelengths, or larger errors (tens of percent) in the transition strengths can make the task more difficult or even impossible to achieve [3]. The lack of atomic data has led to a number of computations of weakly ionised r-process opacities, primarily focussing on lanthanides, being published in recent years. Nevertheless, if the merging process results in the ejection of material with an electron fraction (Y_e) of 0.15 or less, nucleosynthesis should progress to actinides, which are projected to possess photon opacities similar to, or perhaps higher than, lanthanides [4,5]. Moreover, large discrepancies can still be found in the opacities, which are related to the uncertainty of the atomic data produced using different methodologies. [5]
To address this issue, we have developed an optimization procedure to provide atomic data (energy levels and oscillator strengths) that is consistent with available experimental data. The Flexible Atomic Code software package [6] is used, as it allows for the calculation of both radiative and collisional processes. We investigate how this optimization technique affects our calculations as well its impact on line-by-line and grey opacity data. The goal is to provide a more reliable, while still complete, set of atomic data for relevant lanthanides and actinides in the expanding ejecta.

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