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Energy levels structure of Pr II - Gd II ions

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Synopsis Observations of a kilonova associated with GW170817 provide a unique opportunity to study heavy element synthesis in the universe. However, the atomic data of r-process elements are not yet complete enough to decipher the light curves and spectral features of kilonovae. We performed extended atomic calculations for singly ionized elements with $Z = 59 - 64$, by employing GRASP2K package. These computations are based on strategies of Nd II published in [1]. Accuracy of data is evaluated by comparing computed energy levels with the NIST database and other authors.

The calculations were done using multi-configuration Dirac-Hartree-Fock (MCDHF) and configuration interaction (RCI) methods [2, 3], which are implemented in the general-purpose relativistic atomic structure package GRASP2K [4]. The transverse-photon (Breit) interaction, the vacuum polarization, and the self-energy corrections were included in the RCI calculations. Energy levels were computed for states of the configurations: [Xe]$4f^{N-1}5d6s$, [Xe]$4f^{N-1}5d6p$, [Xe]$4f^{N-1}6s6p$, [Xe]$4f^{N-1}5d^2$, [Xe]$4f^N6s$, [Xe]$4f^N6p$ and [Xe]$4f^N5d$, where $N = 3 - 8$ for Pr-Gd ions respectively. For Sm II and Eu II calculations were performed also for states of [Xe]$4f^{N+1}$ configuration, for Gd II were added states of [Xe]$4f^{N-1}6s^2$ configuration. Energy levels were computed up to 10 eV limit for opacity computation of neutron stars merger one day after event.

The configuration space was increased step by step with increasing the number of layers. The orbitals of previous layers were held fixed and only the orbitals of the newest layer were allowed to vary. Sets of virtual orbital were generated by single (S), double (SD) or triple (SDT) substitutions. SDT substitutions were used to generate active space for configuration [Xe]$4f^{N+1}$, SD for [Xe]$4f^N\{6s, 5d, 6p\}$ and S for [Xe]$4f^{N-1}\{5d6s, 5d6p, 6s6p\}$ and [Xe]$4f^{N-1}\{6s^2, 5d^2\}$. The largest active space used in the computations was {8s, 8p, 7d, 6f, 5g}. Substitutions were done only from valence orbitals. Each configuration were computed separately.

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Figure 1 shows the distribution of the energy level number over the relative difference compared to NIST for Sm II, as example. Data for other ions and it's accuracy will be also presented in the abstract.

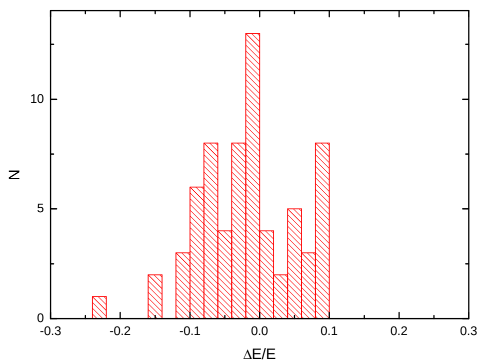

Figure 1. Distribution of the energy levels (N) according the disagreement with NIST database for Sm II.

The analysis of the results shows, that energy levels is suitable for computation opacity of neutron stars merger.

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