Relativistic Hartree-Fock and Dirac-Hartree-Fock calculations of radiative rates in the La I spectrum

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Radiative parameters have been calculated for 392 lines of neutral lanthanum atom in the spectral range from the near ultraviolet to the mid infrared. They were obtained using two different theoretical methods based on the pseudo-relativistic Hartree-Fock (HFR) and the fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) approaches, both including the most important intravalence and core-valence electron correlations. The quality of these radiative parameters was assessed through detailed comparisons between the results obtained using different physical models and between our theoretical results and the experimental data, where available.

Motivations

The determination of radiative parameters in lanthanide atoms and ions has been the subject of many experimental and theoretical studies over the past few decades. This is mainly due to the fact that the remarkably rich spectra corresponding to the first ionization stages of these elements provide useful information for the development of other scientific fields, such as astrophysics and the lighting industry, as mentioned in numerous papers (see e.g. [1-5]). More specifically, in the study of neutron star mergers through gravitational waves, the knowledge of lanthanide spectra is very important. Neutral lanthanum, La I (Z = 57), is characterized by the $5d6s^2\ ^2D_{3/2}$ ground level, while, the lowest excited levels belong to many different configurations such as $5d6s^2$, $5d^26s$, $5d^3$, $4f6s6p$, $5d^27s$, $5d6s7s$, for the even parity, and $5d6s6p$, $5d^26p$, $4f5d6s$, $6s^26p$, $4f6s^2$, for the odd parity, according to the NIST database [6]. The overlap of these configurations is responsible for the strong mixing of most energy levels, which makes both experimental and theoretical analyses very difficult. This notably explains why the designation of some low-lying La I levels is still uncertain or even not yet assigned.

Theoretical methods used

The first computational procedure used in the present work for modelling the atomic structure and calculating the radiative parameters in La I was the pseudo-relativistic Hartree-Fock (HFR) method, originally introduced by Cowan [7] and modified for taking core-polarization effects into account, giving rise to the so-called HFR+CPOL method [8-9]. Three different HFR+CPOL physical models were employed in the calculations. In order to assess the reliability of the pseudo-relativistic Hartree-Fock computations, another theoretical method used in our work was the one implemented in the GRASP2K computer package [10] which uses the fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) method [11] where, in addition to intravalence correlation out of the $5s^25p^6$ closed subshells, the most important core-valence correlations were considered by including the 5p → 4f, 5s → 5d single excitations, and

the $5p^2 \rightarrow 5d^2$, $5s^2 \rightarrow 4f^2$, 5s5p $\rightarrow$ 4f5d double excitations within the relativistic configuration interaction (RCI) approximation.

Results

New oscillator strengths and transition probabilities for 392 spectral lines of neutral lanthanum were obtained in this work. The accuracy of the results was estimated to be better than a factor of two for the entire set of transitions and likely within 30% for many of them. This was assessed from detailed comparisons between different theoretical models based on the HFR and the MCDHF methods, on the one hand, and between the theoretical results and the available experimental data, on the other hand. Among the La I lines listed in the present paper, about 60% have *gf*- and *gA*-values determined for the first time. These new atomic data are expected to be very useful for future astrophysical studies, such as those focused on the neutron star mergers.

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