Ce^{3+} jono energijos spektro ir radiacinių šuolių teorinis tyrimas

Theoretical study of energy spectra and radiative transitions of Ce^{3+} ion

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Observations of gravitational waves from the neutron star merger GW170817 and its electromagnetic counterpart (AT2017gfo) opened a new route to study the origin of heavy elements in the Universe.

Observed properties of AT2017gfo at ultraviolet, optical, and infrared wavelengths are found to be consistent with theoretically expected "kilonova", thermal emission powered by radioactive decays of newly synthesized *r*-process elements. This agreement indicates that *r*-process synthesis takes place in the neutron star merger.

The properties of kilonovae are mainly determined by the chemical compositions in the ejected material as well as its mass and velocity. In particular, lanthanide elements play important role in shaping the light curve and spectra of a kilonova, as these elements have high opacities. To have a better link between the emission properties of a kilonova and nucleosynthesis, it is important to establish accurate atomic opacities. As it is difficult to derive experimental data for the opacity.

In this work, *ab-initio* atomic calculations for triply ionized Ce (Ce^{3+}) were performed. GRASP2018 [1] package, based on the multiconfiguration Dirac-Hartree-Fock and relativistic configuration interaction methods, as well as HULLAC [2] code based on a parametric potential method were used to compute energy spectra and transition data.

Energy spectrum is calculated for the 225 levels for the Ce^{3+} ion. Energy levels are compared with recommended values from the NIST Atomic Spectra Database (ASD) [3] and other available works. The comparison of computed (with GRASP2018 and HULLAC codes) energy levels and other theoretical studies [4,5] with the NIST data giving the difference (in cm^{-1}) $\Delta E = E_{NIST} - E_{calc}$ is presented in Table 1.

As we can see from the Table, computed energies of GRASP2018 agree well with recommended values from the NIST ASD. The rms deviations obtained for energy levels of the $[Kr]4d^{10}5s^25p^6nl$ configurations from the NIST data are 1270 cm^{-1}. The HULLAC energy levels in comparison with the NIST data are too high, and the rms deviations from the NIST data are 5780 cm^{-1}. When comparing the results of other theoretical investigations [4] and [5] with the NIST ASD, the rms deviations are 2160 cm^{-1} and 2240 cm^{-1}, respectively; those authors investigated only low-lying levels.

The NIST ASD specifies one energy value (225625 cm^{-1}) for the two unresolved levels of the $[Kr]4d^{10}5s^25p^65g$ configuration. When comparing this energy level with other works, the level with the lower energy was compared. In the case of GRASP2018 results, the lower energy belongs to the level with J=7/2, while in the case of HULLAC, the lower level has - J=9/2.

The accuracy of the wave functions and transition parameters is evaluated by analyzing the dependencies of the line strength S on the gauge parameter G. The computed transition data are compared with other theoretical computations, too. The evaluation of transition data in details would be presented during the conference.

Table 1. Comparison of energy levels from the present work and other theoretical studies with NIST ASD [3] (deviations in cm^{-1}).

Level	[3]	GRASP	HULLAC	[4]	[5]
4f $^2F^o_{7/2}$	2253	200	172	39	66
5d $^2D_{3/2}$	49737	2084	-361	2174	2202
5d $^2D_{5/2}$	52226	2063	-300	2080	2260
6s $^2S_{1/2}$	86602	571	-6651	2024	2596
6p $^2P^o_{1/2}$	122585	776	-6661	2104	2571
6p $^2P^o_{3/2}$	127292	896	-6278	2156	2591
6d $^2D_{5/2}$	177198	962	-6250	2126	
6d $^2D_{3/2}$	178913	3418	-4550	3121	
7s $^2S_{1/2}$	183502	564	-5077	2326	
5f $^2F^o_{5/2}$	184545	632	-8115		
5f $^2F^o_{7/2}$	184746	579	-7885		
7d $^2D_{3/2}$	221661	198	-6565		
7d $^2D_{5/2}$	221838	-114	-6782		
8s $^2S_{1/2}$	225128	-9	-5990		
5g $^2G_{7/2,9/2}$	225625	159	-5724		

Keywords: energy spectra, transition data, opacity.

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