Accurate calculations of transition energies in doubly ionized Carbon ion (C III)

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In this work, we present benchmark variational calculations for the ground and 15 lowest bound excited ^1S and ^1P states of doubly ionized Carbon (C III). The nonrelativistic wave function of each of these states is generated in an independent calculation by expanding it in terms of a large number (8,000−12,000) of all-electron explicitly correlated Gaussian functions (ECG) who's nonlinear parameters are extensively optimized. A finite nuclear mass value is used in the calculations and the motion of the nucleus is explicitly included in the zero-order nonrelativistic Hamiltonian. The leading relativistic and quantum electrodynamics (QED) corrections to the energy levels are subsequently computed using the perturbation theory. The obtained energies and corrections allow us to determine highly accurate interstate transition frequencies for all naturally occurring stable carbon isotopes ($^{12}C^{++}$, $^{13}C^{++}$, and $^{14}C^{++}$) as well as for the model ion with an infinitely heavy nucleus, $^{\infty}C^{++}$.

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