

Abstract Submitted
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Electric Quadrupole Moments of Metastable States of Ca^+ , Sr^+ , and Ba^+ DASHA JIANG, BINDIYA ARORA, MARIANNA SAFRONOVA, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716-2570, USA — Electric quadrupole moments of the metastable $nd_{3/2}$ and $nd_{5/2}$ states of Ca^+ , Sr^+ , and Ba^+ are calculated using the relativistic all-order method including all single, double, and partial triple excitations of the Dirac-Hartree-Fock wave function to provide recommended values for the cases where no experimental data are available. The contributions of all non-linear single and double terms are also calculated for the case of Ca^+ for comparison of our approach with the CCSD(T) results. The third-order many body perturbation theory is used to evaluate contributions of high partial waves and the Breit interaction. The remaining omitted correlation corrections are estimated as well. Extensive study of the uncertainty of our calculations is carried out to establish accuracy of our recommended values to be 0.5% - 1% depending on the particular ion. Comprehensive comparison of our results with other theoretical values and experiment is carried out. Our result for the quadrupole moment of the $3d_{5/2}$ state of Ca^+ ion, $1.849(17) ea_0^2$, is in agreement with the most precise recent measurement $1.83(1) ea_0^2$ by Roos et al. [Nature 443, 316 (2006)].

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