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Relativistic all-order calculations of Th, Th⁺ and Th²⁺ atomic properties ULYANA SAFRONOVA, University of Nevada, Reno, MARIANNA SAFRONOVA, University of Delaware and JQI, NIST and the University of Maryland, CHARLES W. CLARK, JQI, NIST and the University of Maryland — Excitation energies, term designations, and q-factors of Th, Th⁺ and Th²⁺ are determined using a relativistic hybrid configuration interaction (CI) + all-order approach that combines configuration interaction and linearized coupled-cluster methods. The results are compared with other theory and experiment where available. Good agreement with experiment was found even for neutral Th owing to all-order treatment of the dominant correlation corrections and sufficient saturation of the configuration space. We find some "vanishing" q-factors, similar to those known in lanthanide spectra. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for Th²⁺. To estimate the uncertainties of our results, we compared our values with the available experimental lifetimes for higher $5f7p^{3}G_{4}$, $7s7p \ ^3P_0$, $7s7p \ ^3P_1$, and $6d7p \ ^3F_4$ levels of Th²⁺. These calculations provide a benchmark test of the CI+all-order method for heavy systems with several valence electrons and yield recommended values for transition rates and lifetimes of Th²⁺.

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