ELECTRONIC STRUCTURE OF THE GROUND AND EXCITED STATES OF EUROPIUM OXIDE (EuO)

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Despite being subject to numerous single reference computations, Europium Oxide (EuO) to date has not had its electronic structure studied with multireference methods. High-level ab initio approaches were performed detailing its numerous excited states, and spin multiplicities. Complete active space self-consistent field (CASSCF) and multireference configuration interaction (MRCI) was utilized to compute the ground and excited state properties of EuO. The potential energy curves for the ground, excited states, and different dissociation channels are explored. Spin-orbit corrections were performed with the Breit-Pauli hamiltonian. When available comparisons to experiment are made.