THE ELECTRONIC STRUCTURE OF THE PLUTONYL ION

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Restricted Hartree-Fock (RHF) and spin-orbit configuration-interaction (SOCI) calculations were performed on the ground and low-lying excited states of the 1+ plutonyl ion, PuO_2^{1+}. These results are compared to previous results on the 2+ plutonyl ion, PuO_2^{2+}. The low energy transitions are f→f, additionally, ligand-to-metal charge transfer (LMCT) states are studied. Recently, intensity spectra are obtainable using these methods. Our results will be compared to experiment.