

THE ENERGY LEVELS OF URANIUM IONS DOPED INTO CALCIUM FLUORIDE

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Uranium ions in CaF₂ crystals have been studied extensively via electron paramagnetic resonance and optical spectroscopy. Various valencies and charge compensation mechanisms have been claimed. Ab initio spin-orbit configuration interaction calculations are performed on these systems. The primary properties of interest are the energy levels and magnetic moments. The CaF₂ host is modeled with a large finite cluster of ions which approximate the Madelung potential of the crystal lattice. Uranium is modeled with relativistic effective core potentials and Gaussian cc-pVDZ basis sets. As an indication of accuracy it is noted that the best calculations on the U⁴⁺ free ion have a maximum relative error of 9.6% when compared to the experimental spectrum of this 5f² configuration.