THE ENERGY LEVELS OF LANTHANIDE IONS, FREE AND DOPED INTO CALCIUM FLUORIDE

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Lanthanide ions, both free and in CaF_2 crystals, have been studied extensively via optical spectroscopy and electron paramagnetic resonance. Ab initio spin-orbit configuration interaction calculations are performed on some of these systems. The primary properties of interest are the energy levels and magnetic moments. The CaF_2 host is modeled with a large finite cluster of ions which approximate the Madelung potential of the crystal lattice. Lanthanide ions are modeled with relativistic effective core potentials and Gaussian cc-pVDZ basis sets. The results for the lanthanide ions are compared and contrasted with similar studies on actinide ions.