GROUND-STATE SPLITTINGS OF ACTINIDE IONS IN CaF_2

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The energy-level splittings of Am^{2+}, Cm^{3+}, Es^{2+}, Pu^{3+}, and U^{4+} in an octahedral site of CaF_2 were studied using restricted Hartree-Fock and spin-orbit configuration-interaction calculations. The CaF_2 host was modeled with a large finite cluster of ions which approximate the Madelung potential of the crystal lattice[a]. The actinide dopants were treated with relativistic effective core potentials and Gaussian correlation consistent double-zeta plus polarization basis sets. The primary properties of interest are energy splittings and magnetic moments.

[a]N. W. Winter, M. Ross and R. M. Pitzer *J. Phys. Chem.* **94**, 1172 (1990).