GROUND-STATE SPLITTING OF Am^{2+} IN CaF_2

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The energy-level splittings of the $5f^7$ nominal $^8S_{7/2}$ ground-state of Am^{2+} in an octahedral site of CaF_2 were studied using *ab initio* quantum chemical methods. The CaF_2 host was modeled with a large finite cluster of ions which approximate the Madelung potential of the crystal lattice[a]. The potential energy curve for the symmetric stretch of the nearest-neighbor fluoride ions was calculated. The actinide dopant was treated with relativistic core potentials and Gaussian double-zeta basis sets.

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