

Investigating Complexation-Induced Chirality in Ln(III) and An(III)-3,4,3-LI(1,2-HOPO) Small Molecule and Siderocalin Protein Complexes

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The solid-state interactions between the octadenate siderophore analogue 3,4,3-LI(1,2-HOPO) and trivalent Ln(III) and An(III) cations were investigated via single-crystal and protein crystallography. The ability to directly compare single crystal and protein crystal structures is unprecedented, and herein we highlight protein-induced chirality in a series of twelve Ln-HOPO-siderocalin (Ln=La-Lu, except Ce) macromolecular complexes, which contrasts with the ten centrosymmetric Ln-HOPO (Ln=Nd-Lu) structures (space group *P-1*) observed via single crystal X-ray diffraction. Comparison of small molecule and macromolecular complexes provide unprecedented insights into the biological coordination of heavy radioelements, and inspired by Ln(III) results, initial efforts to extend work to natural (Ac(III)) and synthetic (Es(III)) radionuclides will also be highlighted.