HOMOLEPTIC NINE-COORDINATE An(III) AND Ln(III) COMPLEXES: UNRAVELING F-ELEMENT BONDING

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Oxygen atoms of the nine-coordinate waters in both actinide(III) and lanthanide(III) nonoaquo triflate salts adopt a highly symmetric tricapped, trigonal-prismatic geometry about the metal center. The metal to prismatic water bond lengths in actinide complexes are longer than the lanthanide complexes of similiar ionic radii while the metal to capping water bond lengths are nearly identical. Scalar-relativistic density functional theory calculations have been utilized to further understand this trend. The role of f-electrons in complex formation is discussed.