THEORETICAL DETERMINATION AND ASSIGNMENT OF THE VIBRATIONAL SPECTRA OF ACTINOCENES: $An(\eta^8\text{-}C_8H_8)_2$ (An = Th, Pa, U, Np, Pu, Am)

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Relativistic density functional methods have been used to calculate the optimized geometries and vibrational frequencies of actinocenes, $An(\eta^8\text{-}C_8H_8)_2$ (An = Th, Pa, U, Np, Pu, Am). The influences of scalar and spin-orbit relativistic effects on the geometries and vibrational frequencies of these organoactinide complexes are discussed. The calculated scalar-relativistic vibrational frequencies and absorption intensities are in excellent agreement with experimental results. Clear-cut assignments of all the infrared and Raman vibrational modes of actinocenes are presented.