Experimental UV–vis spectra of the U^{VI} sha and bha systems in aqueous solution (insets), and calculated B3LYP-TD-DFT excitation spectra for both [UO_{2}shaOH_{2}] and [UO_{2}bhaOH_{2}] including the COSMO potential. For comparison calculated B3LYP-TD-DFT excitation spectra for [UO_{2}sha(OH_{2})_{3}]^{+} and [UO_{2}bha(OH_{2})_{3}]^{+} have been reproduced from Ref. 21. Experimental intensities have been scaled to match the calculated intensities of the sha and bha systems’ 395 and 332 nm excitations, respectively. The cusp-like features at ca. 440 and 450 nm in the experimental spectra are baseline correction artifacts.