Figure S1. Single and multiple scattering paths with effective path lengths less than 4.8 Å and intensities at least 2.5% of the path of maximum scattering intensity for the UO_2^{2+}-HDEHP complex with $\theta_p = 155°$.

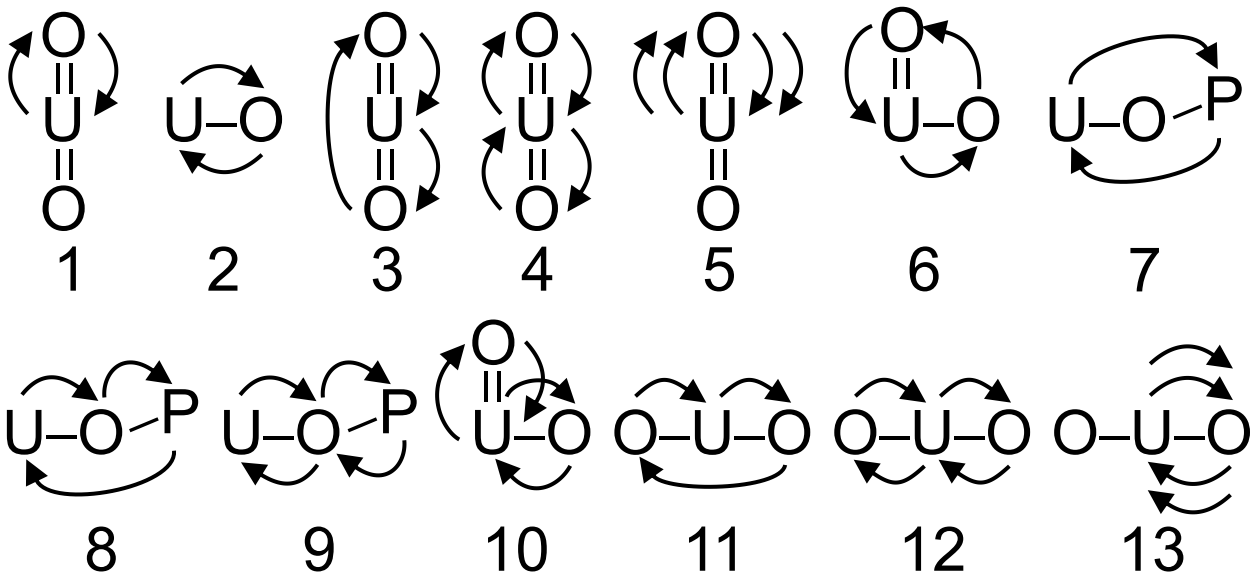

Figure S2. Contribution of each individual FEFF8.00 scattering path to the total fit of the UO_2^{2+}-HDEHP experimental EXAFS for $\theta_p = 155°$. Distances are not phase shift corrected.

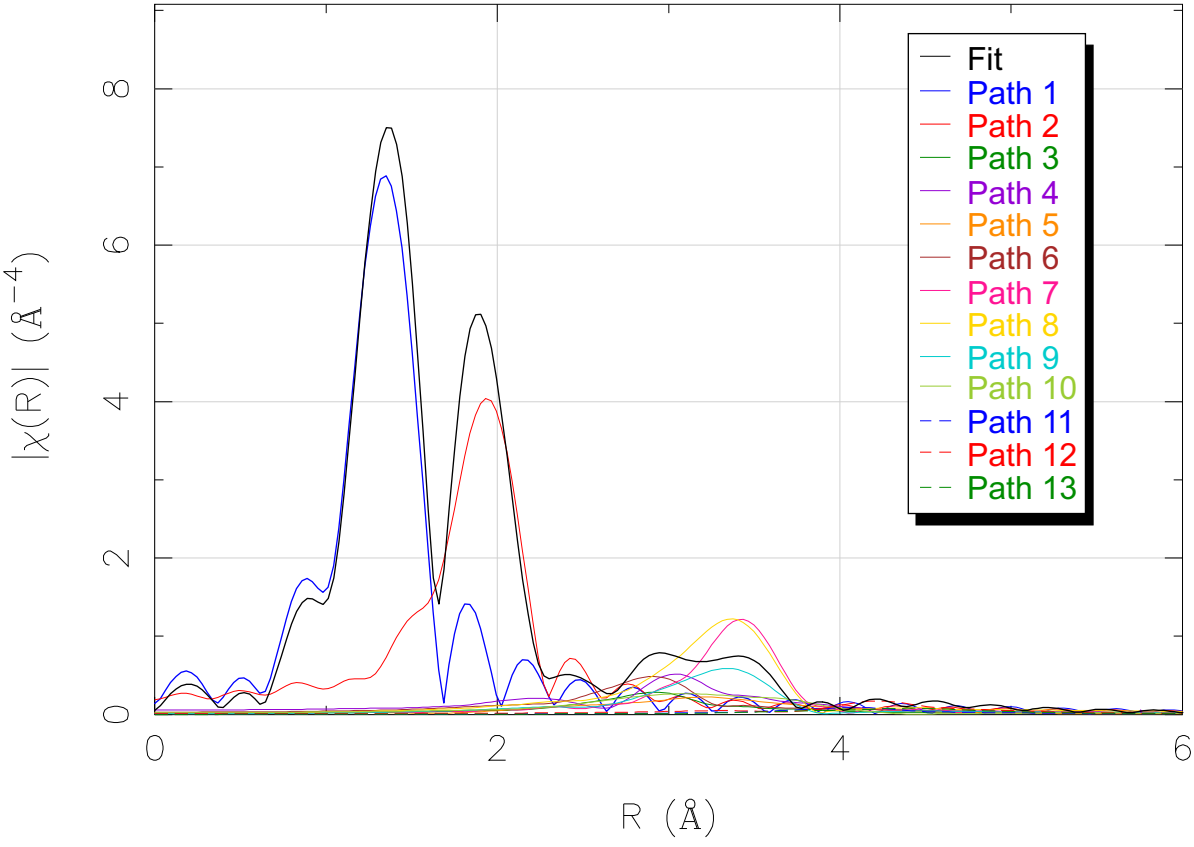

Figure S3. Single and multiple scattering paths with effective path lengths less than 4.8 Å and intensities at least 2.5% of the path of maximum scattering intensity for the Eu-HDEHP complex with $\theta_p = 150°$.

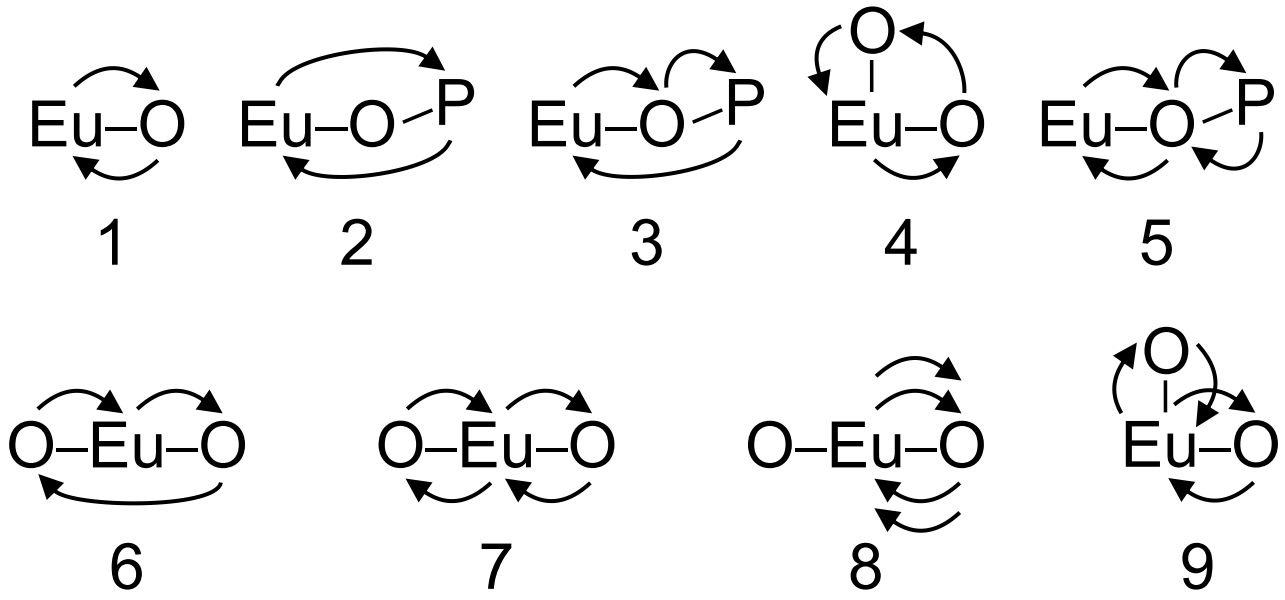

Figure S4. Contribution of each individual FEFF8.00 scattering path to the total fit of the Eu-HDEHP experimental EXAFS for $\theta_p = 150°$. Distances are not phase shift corrected.

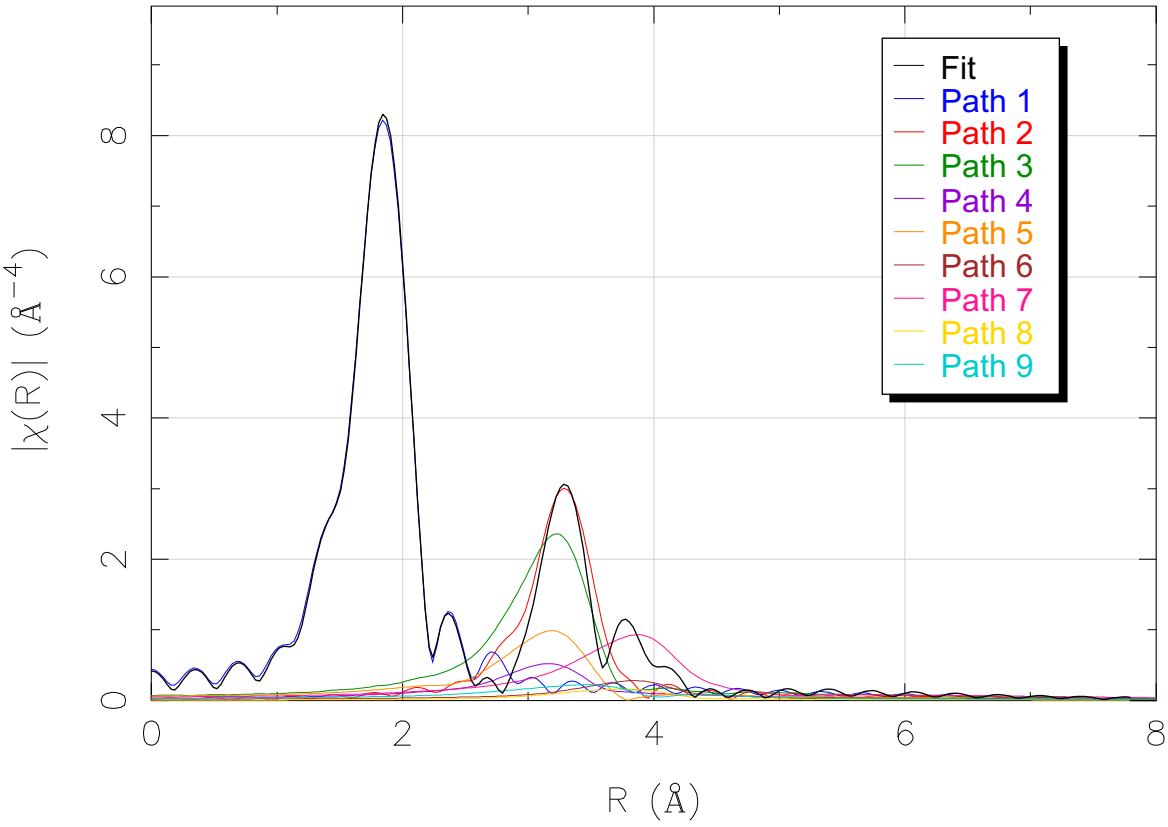

Table S1. Model for fitting the UO_2^{2+}-HDEHP EXAFS to the FEFF8.00 calculated paths. N_O = number of coordinated HDEHP oxygens, R_{yl} = axial "-yl" U=O oxygen distance, R_{eq} = U-O distance for coordinated HDEHP oxygens, R_P = U-P distance, θ_P = ∠U-O-P, $R_{O\text{-}P}$ = O-P distance for the HDEHP oxygen and phosphorous = $(2R_{eq}\cos(\theta_P) \pm [\{2R_{eq}\cos(\theta_P)\}^2 - 4\{R_{eq}^2 - R_P^2\}]^{0.5}) / 2$, σ_{yl}^2 = Debye-Waller factor for axial -yl oxygens, σ_{eq}^2 = Debye-Waller factor for coordinated HDEHP oxygens, σ_P^2 = Debye-Waller factor for phosphorous. Parameters varied in the fit are shown in red. The other parameters were either calculated from the varied parameters, or fixed at the given numeric values.

Path	Coordination Number, N	Effective Path Length, R	Debye-Waller Factor, σ^2
1	2	R_{yl}	σ_{yl}^2
2	N_O	R_{eq}	σ_{eq}^2
3	2	$2R_{yl}$	$2\sigma_{yl}^2$
4	2	$2R_{yl}$	$2\sigma_{yl}^2$
5	4	$2R_{yl}$	$4\sigma_{yl}^2$
6	$4N_O$	$([R_{yl}^2 + R_{eq}^2]^{0.5} + R_{yl} + R_{eq}) / 2$	$\sigma_{yl}^2 + \sigma_{eq}^2$
7	N_O	R_P	σ_P^2
8	$2N_O$	$(R_{eq} + R_P + R_{O\text{-}P}) / 2$	$\sigma_{eq}^2 + \sigma_P^2$
9	N_O	$R_{eq} + R_{O\text{-}P}$	$\sigma_{eq}^2 + \sigma_P^2$
10	$4N_O$	$R_{yl} + R_{eq}$	$\sigma_{yl}^2 + \sigma_{eq}^2$
11	N_O	$2R_{eq}$	$2\sigma_{eq}^2$
12	N_O	$2R_{eq}$	$2\sigma_{eq}^2$
13	N_O	$2R_{eq}$	$4\sigma_{eq}^2$

Table S2. Model for fitting the Eu^{3+}-HDEHP EXAFS to the FEFF8.00 calculated paths. N_O = number of coordinated oxygens, R_O = Eu-O distance, R_P = Eu-P distance, θ_P = ∠Eu-O-P, $R_{O\text{-}P}$ = O-P distance = $(2R_O\cos(\theta_P) \pm [\{2R_O\cos(\theta_P)\}^2 - 4\{R_O^2 - R_P^2\}]^{0.5}) / 2$, σ_O^2 = Debye-Waller factor for coordinated oxygen, σ_P^2 = Debye-Waller factor for phosphorous. Parameters varied in the fit are shown in red. The other parameters were calculated from the varied parameters.

Path	Coordination Number, N	Effective Path Length, R	Debye-Waller Factor, σ^2
1	N_O	R_O	σ_O^2
2	N_O	R_P	σ_P^2
3	$2N_O$	$(R_O + R_P + R_{O\text{-}P}) / 2$	$\sigma_O^2 + \sigma_P^2$
4	$4N_O$	$(2 + \sqrt{2})R_O / 2$	$2\sigma_O^2$
5	N_O	$R_O + R_{O\text{-}P}$	$\sigma_O^2 + \sigma_P^2$
6	N_O	$2R_O$	$2\sigma_O^2$
7	N_O	$2R_O$	$2\sigma_O^2$
8	N_O	$2R_O$	$2\sigma_O^2$
9	$4N_O$	$2R_O$	$2\sigma_O^2$