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Supporting information for article:

Refinement of the uranium dispersion corrections from anomalous diffraction

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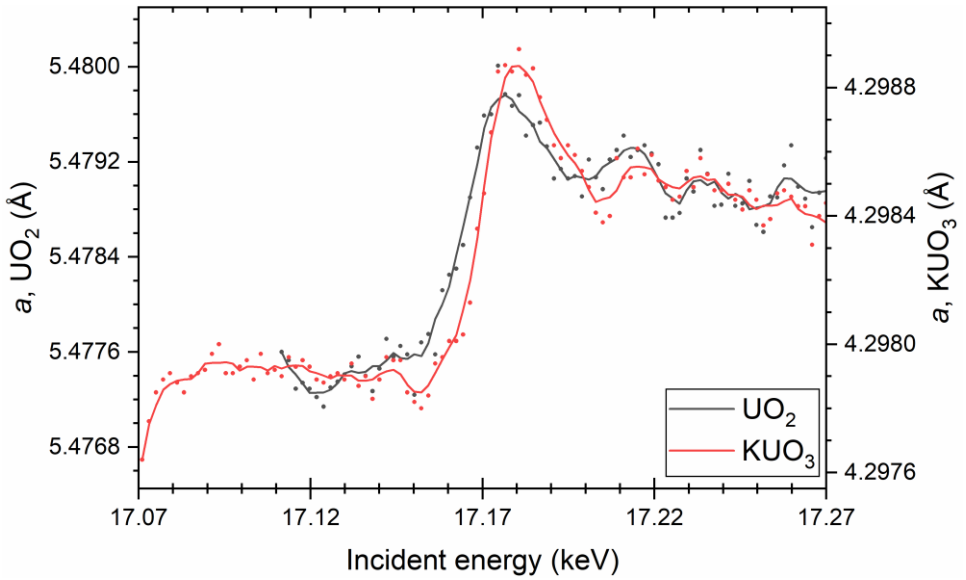

Figure S1. Evolution of the lattice parameter in UO_2 and in KUO_3 during the DAFS acquisition. The data points correspond to the lattice parameter values obtained during the final iteration of the TOPAS refinement. The solid lines represent an adjacent-averaging fit to guide the eye. Both datasets show the typical signature of an U L_3-edge X-ray absorption spectrum. As the absorption increases towards the edge, the sample heats up and consequently, the unit cell expands.

Table S1. Crystallographic properties of KUO_3 (Van den Berghe *et al.*, 2004) and UO_2 (Leinders *et al.*, 2015).

	KUO_3	**UO_2**
Space group (#)	$Pm\bar{3}m$ (221)	$Fm\bar{3}m$ (225)
***a* (Å)**	4.2930 (6)	5.47127 (8)
	Multiplicity, Wyckoff letter	
U	1 *a*	4 *a*
O	3 *d*	8 *c*
K	1 *b*	
	Anisotropic thermal parameters	
U_{11} (U)	0.0137(5)	-
U_{22} (U)	0.0137(5)	-
U_{33} (U)	0.0137(5)	-
U_{11} (O)	0.0139(8)	-
U_{22} (O)	0.0267(5)	-
U_{33} (O)	0.0267(5)	-
U_{11} (K)	0.0242(5)	-
U_{22} (K)	0.0242(5)	-
U_{33} (K)	0.0242(5)	-

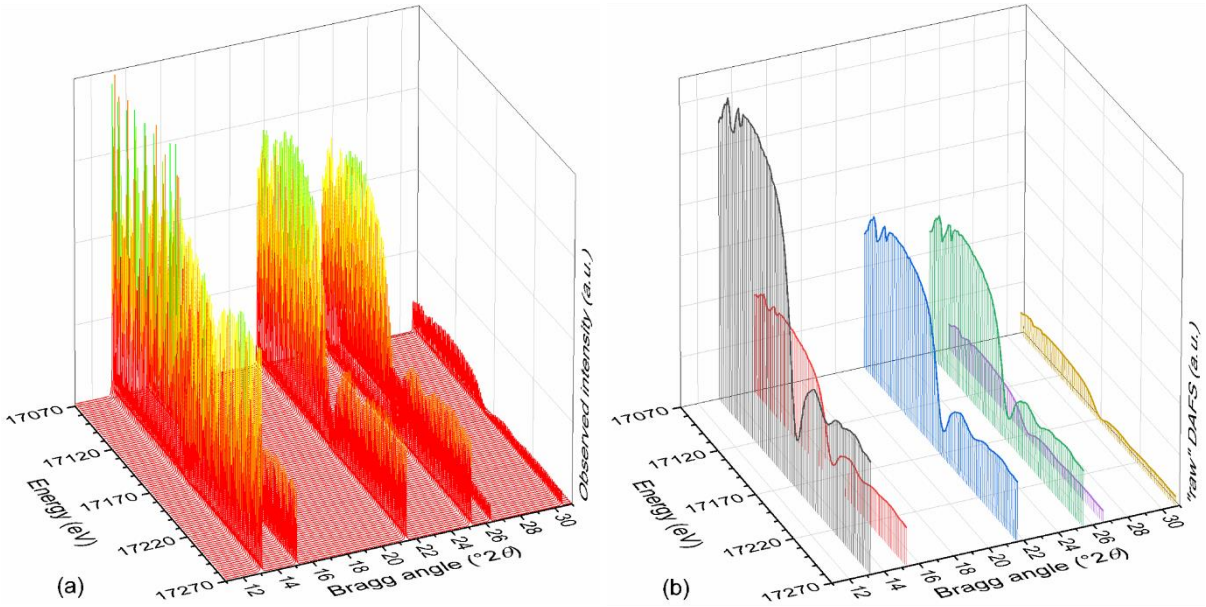

Figure S2. (a) 3D plot of the UO_2 diffraction patterns measured at incident energies between 17.07 and 17.27 keV. (b) 3D plot of the *raw* DAFS spectrum derived for each reflection (straights lines parallel to the *z*-axis are added to guide the eye).

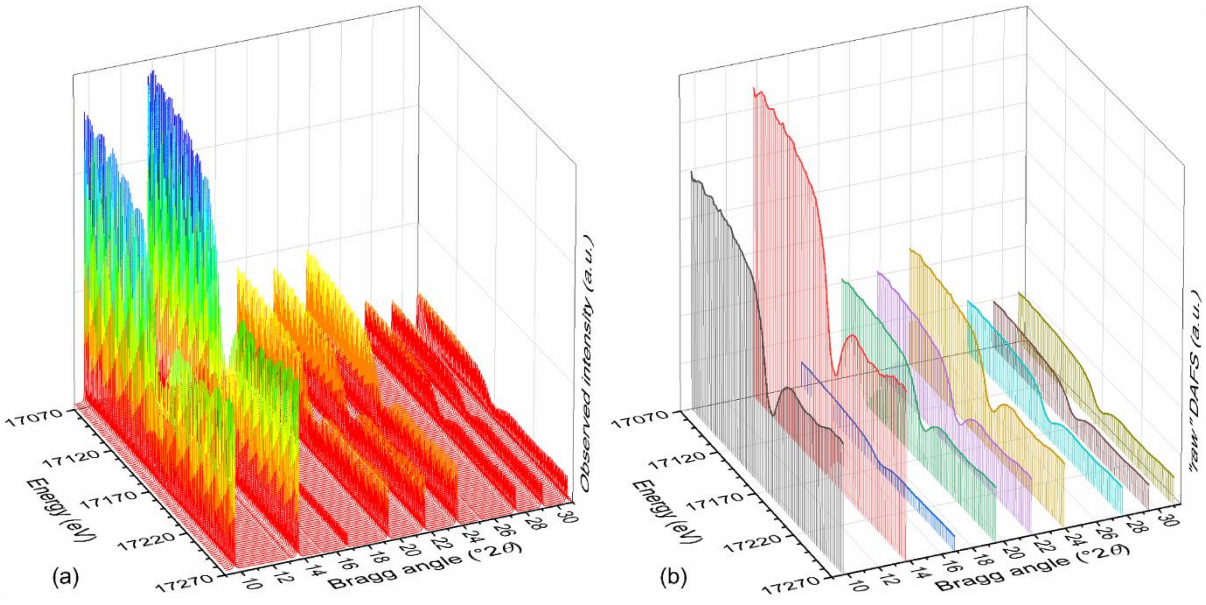

Figure S3. (a) 3D plot of the KUO_3 diffraction patterns measured at incident energies between 17.07 and 17.27 keV. (b) 3D plot of the *raw* DAFS spectrum derived for each reflection (straights lines parallel to the *z*-axis are added to guide the eye).

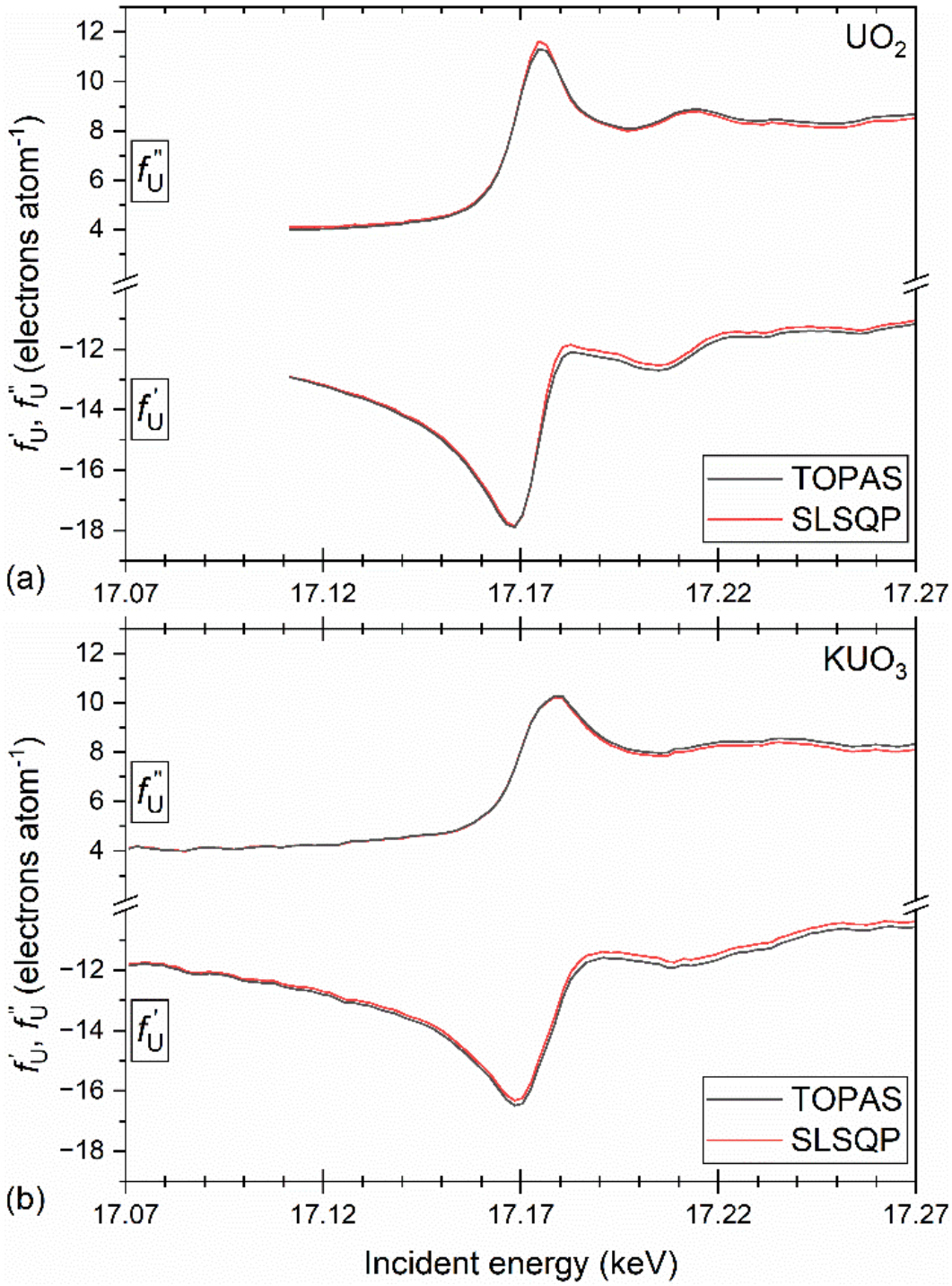

Figure S4. Comparison of the uranium dispersion corrections $f'_U(E_i)$ and $f''_U(E_i)$, resulting from the iterative full-pattern refinement method on the DAFS dataset of UO_2 (a) and KUO_3 (b). A comparison is made to the corresponding values refined using the SLSQP method.

References

Leinders, G., Cardinaels, T., Binnemans, K. & Verwerft, M. (2015). *J. Nucl. Mater.* **459**, 135-142.

Van den Berghe, S., Leenaers, A. & Ritter, C. (2004). *J. Solid State Chem.* **177**, 2231-2236.