

Supplementary Information

A Redox-Innocent Uranium(IV)-Quinoid Metal-Organic Framework

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ACS Omega

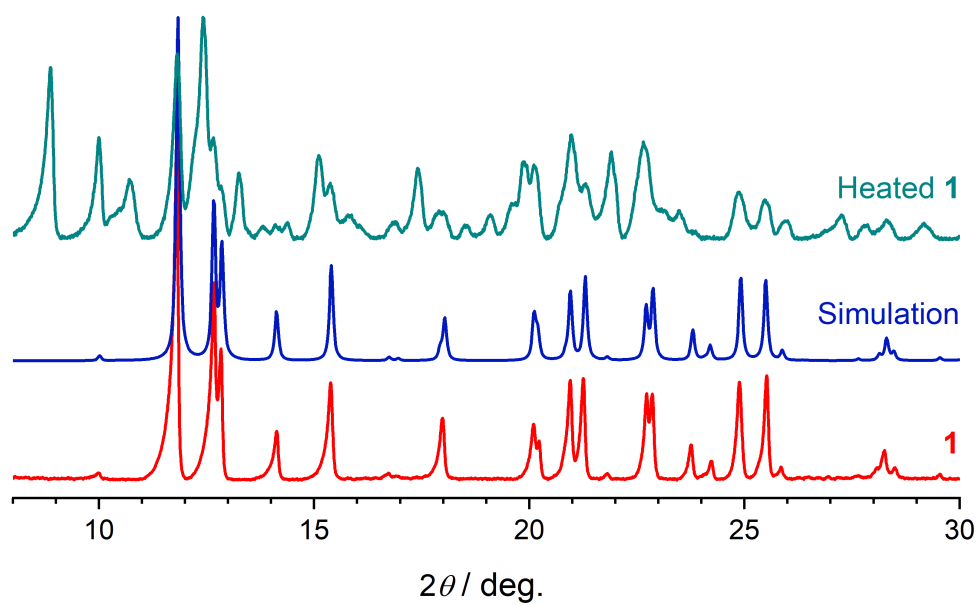


Figure S1. Experimental (red) and simulated (blue) X-ray powder diffractogram of **1** obtained at RT. The turquoise trace is the powder diffractogram of a sample of **1** heated to 100 °C (0.1 K min^{-1}) under a dry dinitrogen atmosphere.

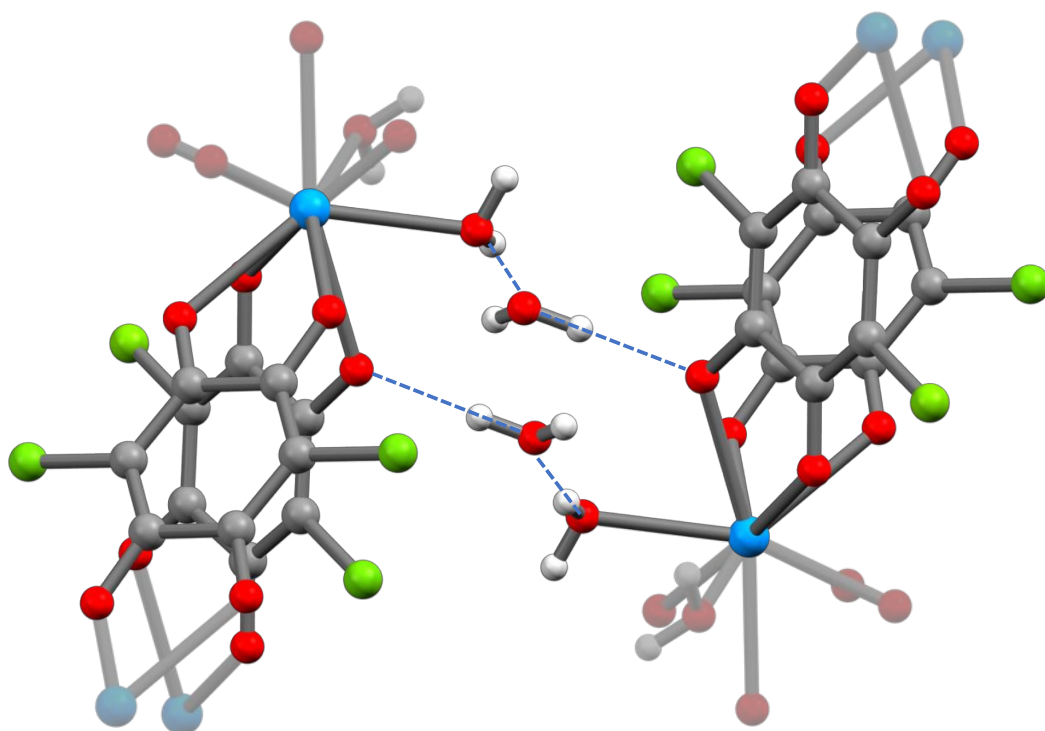


Figure S2. Hydrogen bonding pattern of the inter-pore water molecules in **1**.

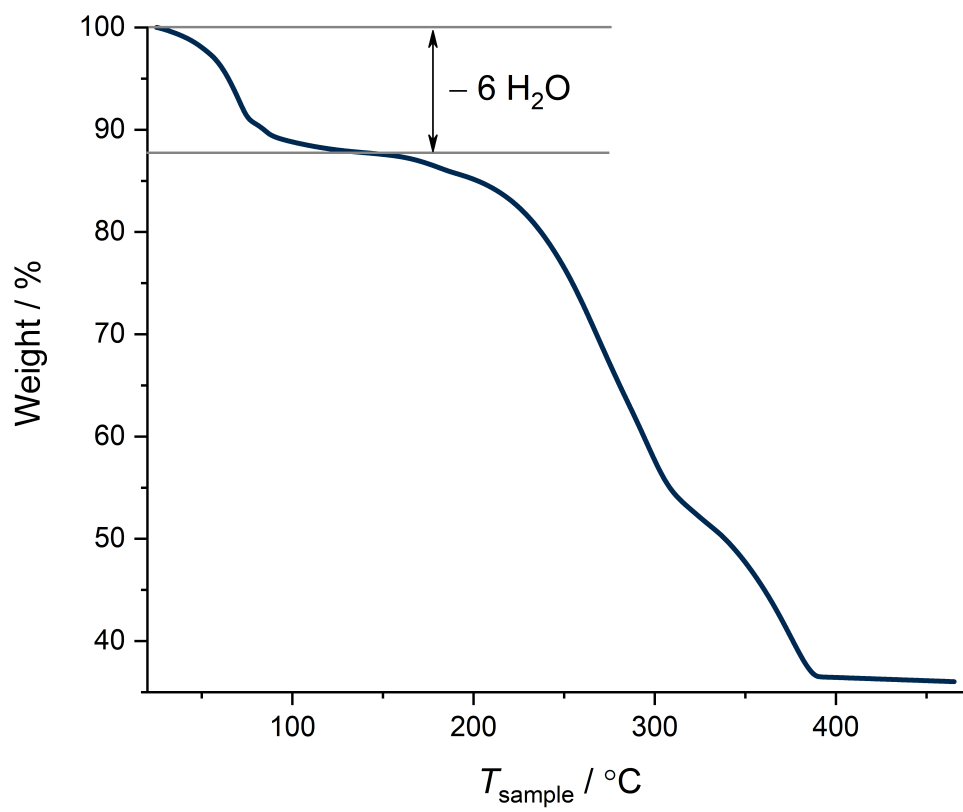


Figure S3. Thermogravimetric analysis of 1.

Table S1. Refinement and crystallographic data of **1** at $T = 285$ K.

<i>CCDC number</i>	1897473
Empirical formula	$C_{12}H_{12}Cl_4O_{14}U$
Formula weight	760.05
Crystal system	monoclinic
Space group	$C2/c$
$a / \text{\AA}$	13.8598(7)
$b / \text{\AA}$	11.4960(6)
$c / \text{\AA}$	12.6100(6)
$\alpha / ^\circ$	90
$\beta / ^\circ$	96.415(5)
$\gamma / ^\circ$	90
$V / \text{\AA}^3$	1996.60(17)
Z	4
$\rho_{\text{calc}} / \text{g cm}^{-3}$	2.528
μ / mm^{-1}	8.737
$F(000)$	1424.0
Radiation	Mo $K\alpha$ ($\lambda = 0.71073 \text{\AA}$)
2θ range for data collection / $^\circ$	5.834 to 59.466
Index ranges	$-16 \leq h \leq 18,$ $-15 \leq k \leq 11,$ $-15 \leq l \leq 17$
Reflections collected	5341
Independent reflections	2422
	$[R_{\text{int}} = 0.0221, R_{\text{sigma}} = 0.0305]$
Data/restraints/parameters	2422/0/148
Goodness of fit on F^2	1.057
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0200, wR_2 = 0.0434$
Final R Indexes [all data]	$R_1 = 0.0221, wR_2 = 0.0445$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.13/−0.83

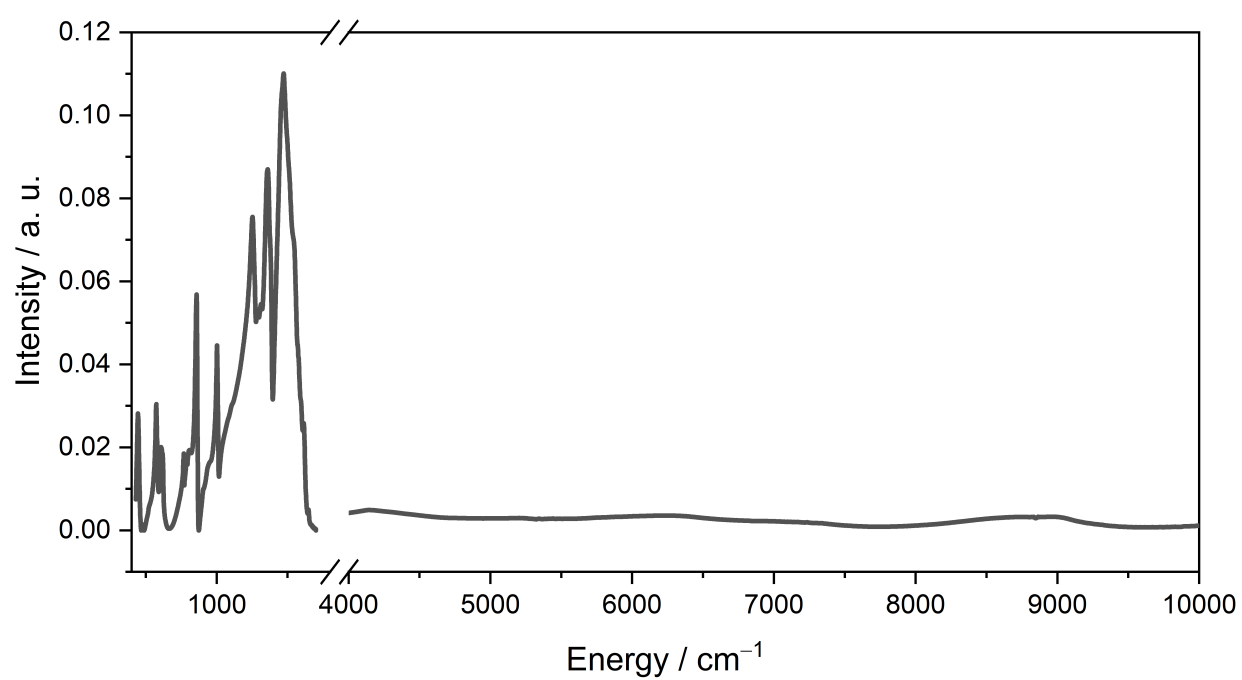


Figure S4. NIR/MIR spectrum of polycrystalline **1** obtained at RT.

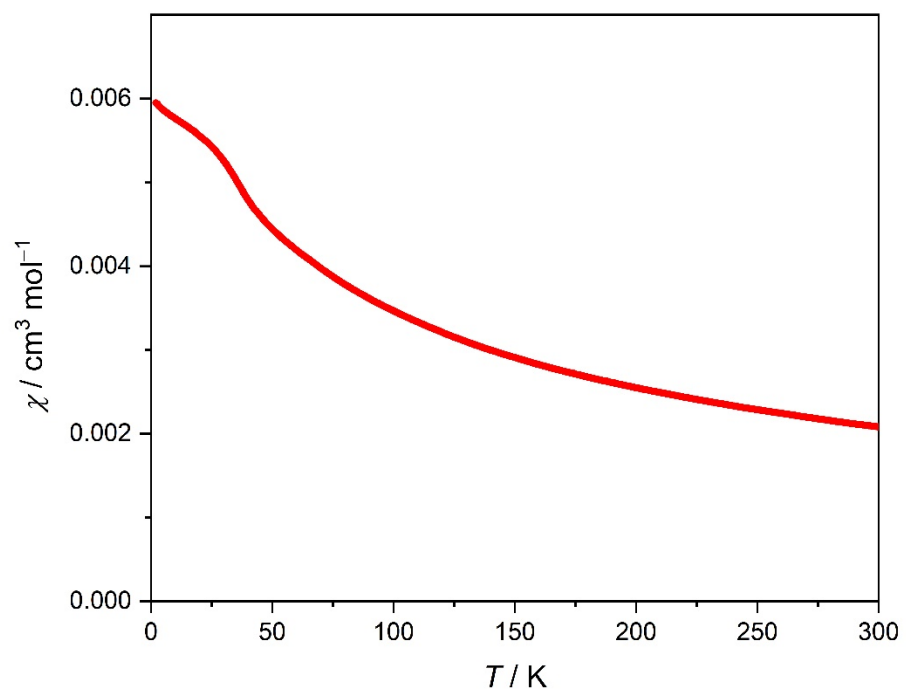


Figure S5. Magnetic susceptibility, $\chi \equiv M/\mu_0 H$, of polycrystalline **1** obtained with $\mu_0 H = 1$ T.

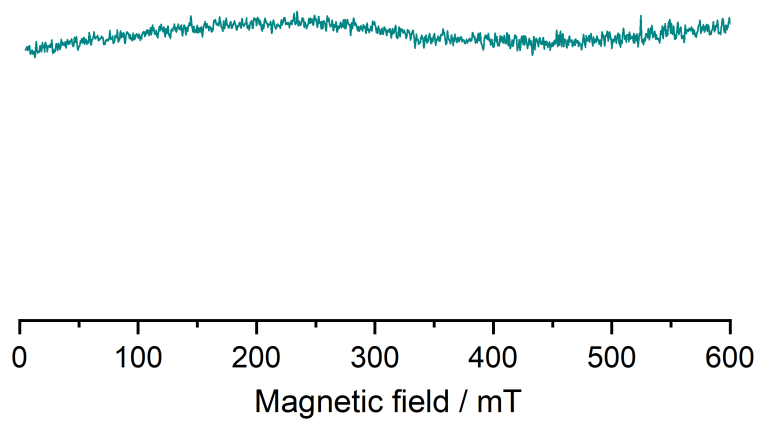


Figure S6. X-band EPR spectrum of polycrystalline **1** obtained at $T = 77$ K.

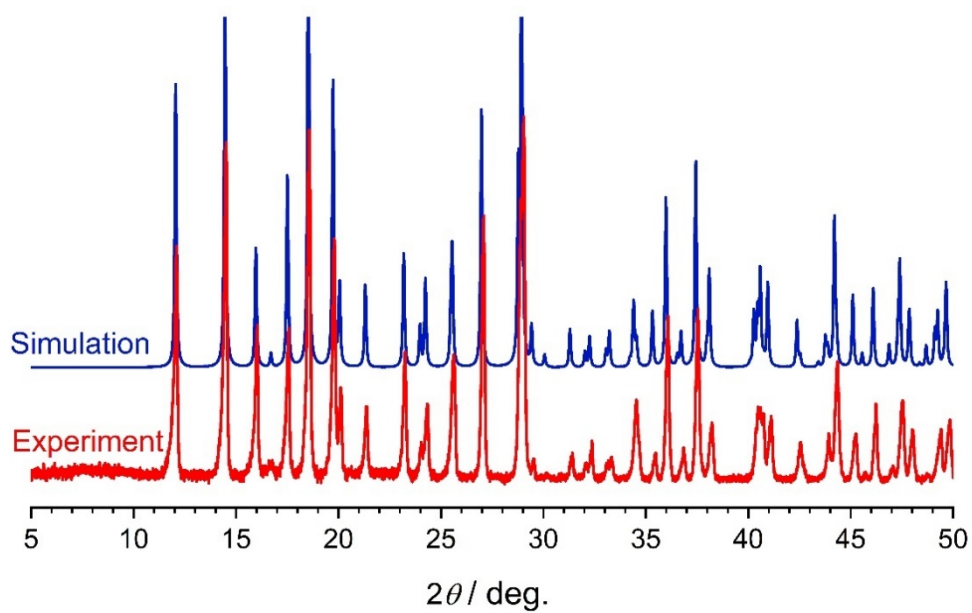


Figure S7. Experimental and simulated X-ray powder diffractogram of $U(SO_4)_2 \cdot 4H_2O$ obtained at RT.

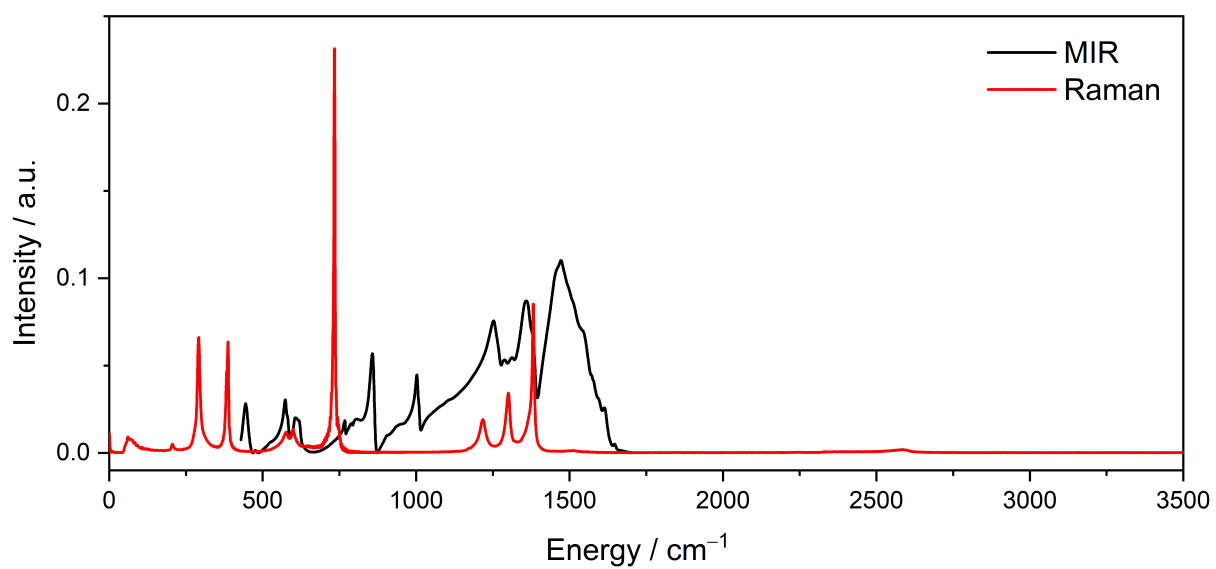


Figure S8. MIR and Raman spectra of polycrystalline **1** obtained at RT.