Electronic Supplementary Information for Dalton Transactions

Probing the local coordination environment and nuclearity of uranyl(VI) complexes in non-aqueous media by emission spectroscopy

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SUPPLEMENTARY INFORMATION

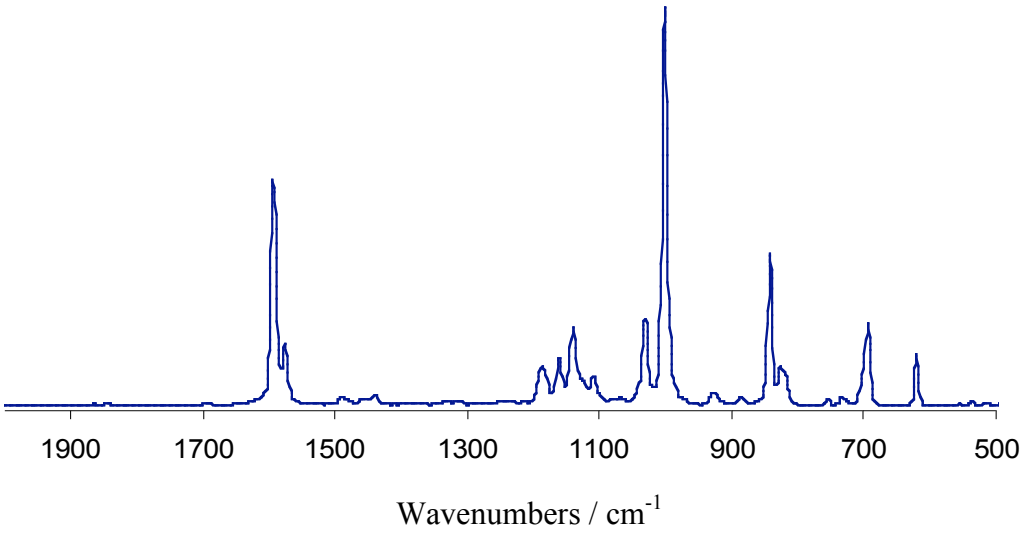

Figure S1. Raman spectrum (in absorbance) between 2000–500 cm^{-1} of crystalline $[UO_2(TPIP)_2(THF)]$ (**4**).

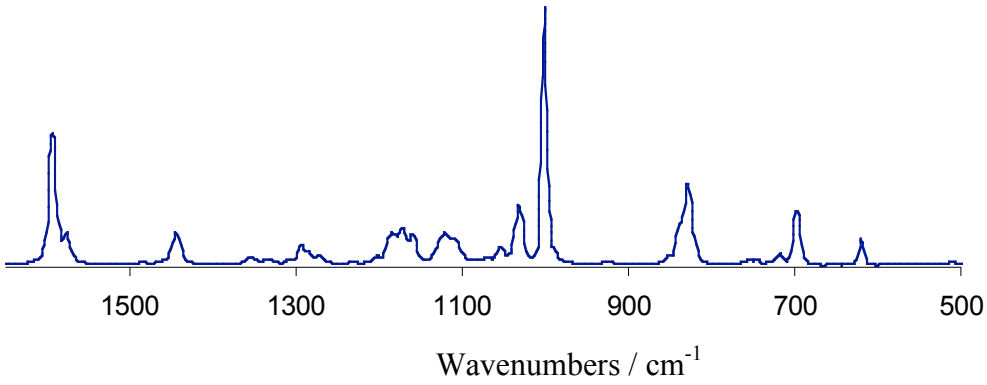

Figure S2. Raman spectrum (in absorbance) between 1650–500 cm^{-1} of crystalline $[UO_2(TPIP)_2(OPCy_3)]$ (**5**).

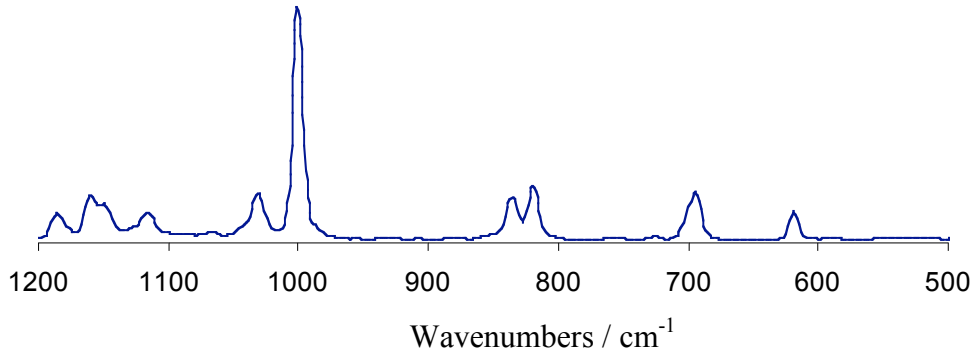

Figure S3. Raman spectrum (in absorbance) between 1200–500 cm^{-1} of powdered $[UO_2(TPIP)_2]_3$ (**7**)

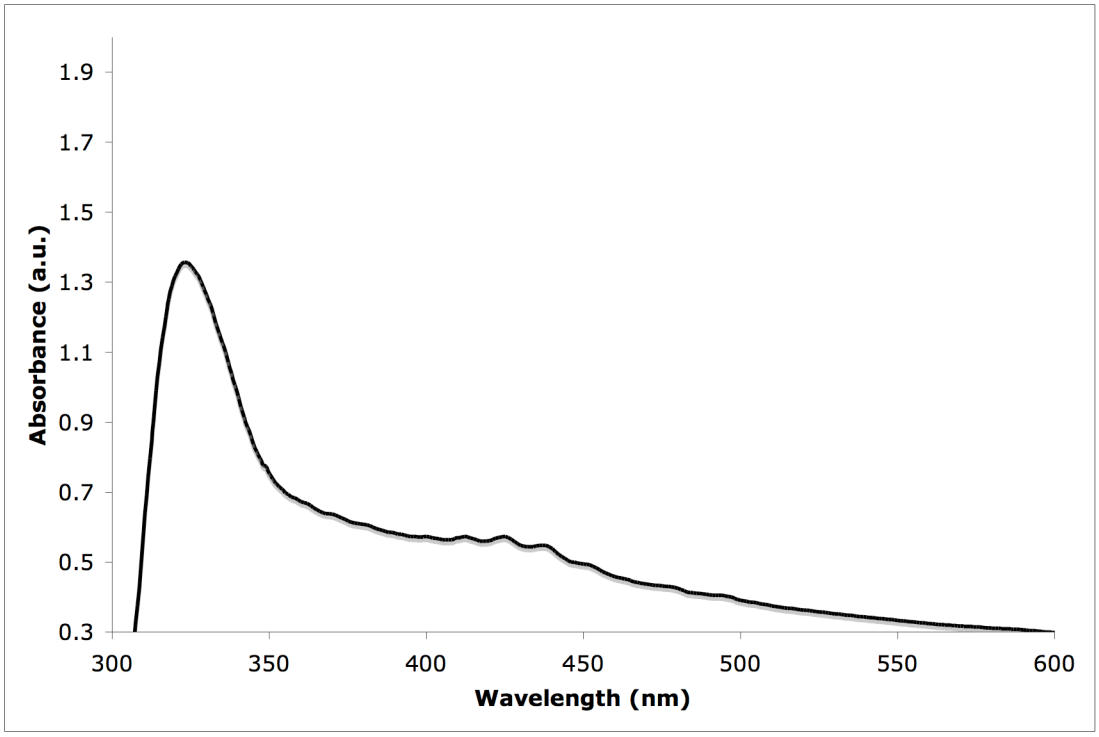

Figure S4. UV-vis spectrum of $[UO_2Cl_2(Ph_3AsO)]$ (**2**) in CH_2Cl_2 (295 K)

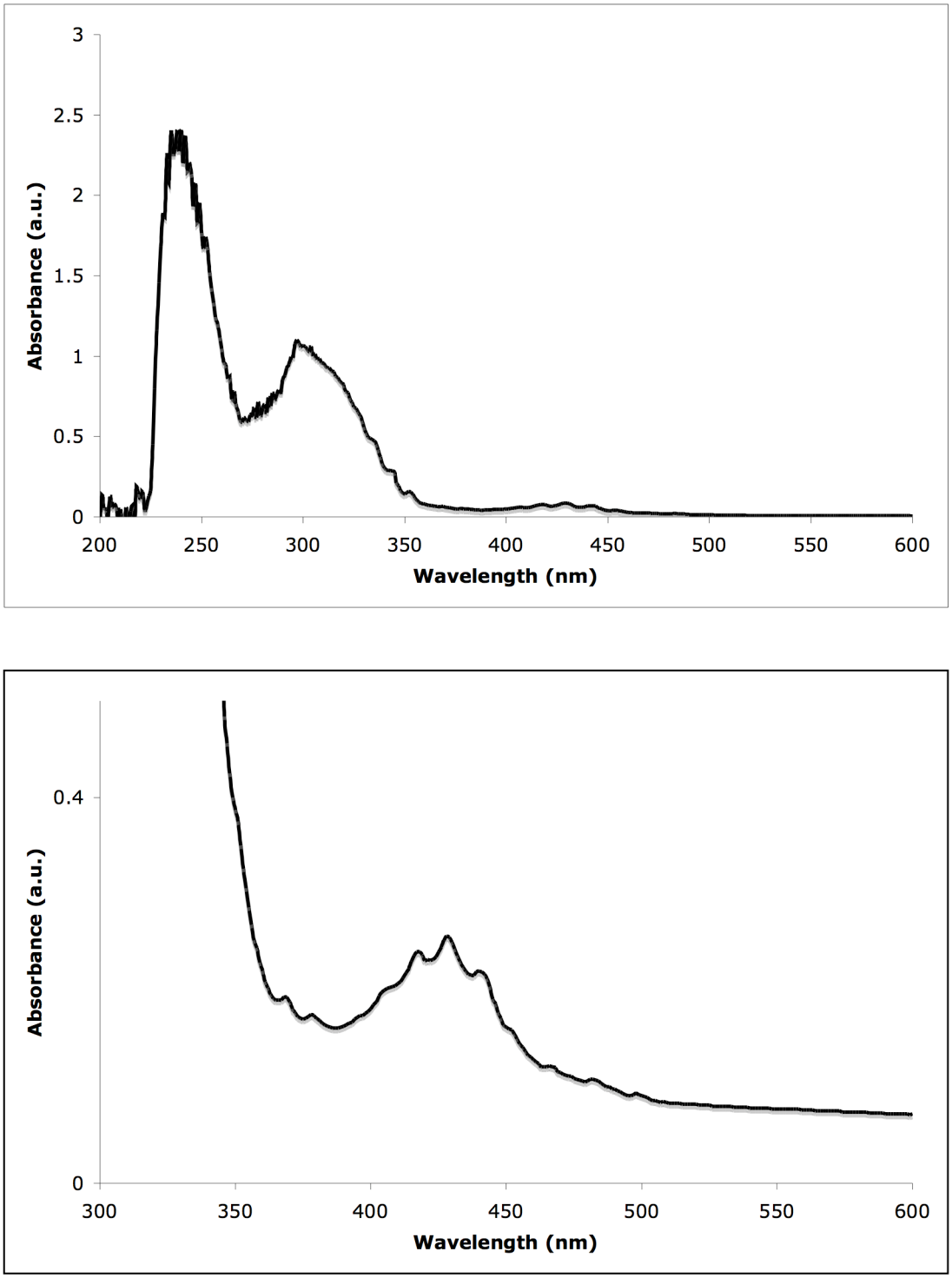

Figure S5. UV-vis spectrum of $[UO_2(TPIP)_2(thf)]$ (**4**) in CH_2Cl_2 (295 K)

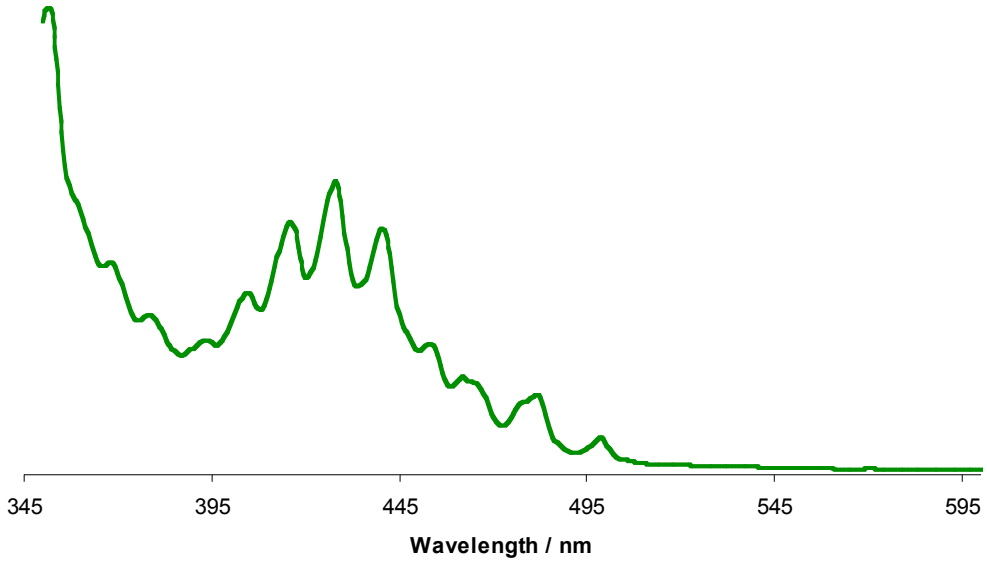

Figure S6. UV-vis spectrum of $[UO_2(TPIP)_2(Cy_3PO)]$ (**5**) in CH_2Cl_2 (295 K)

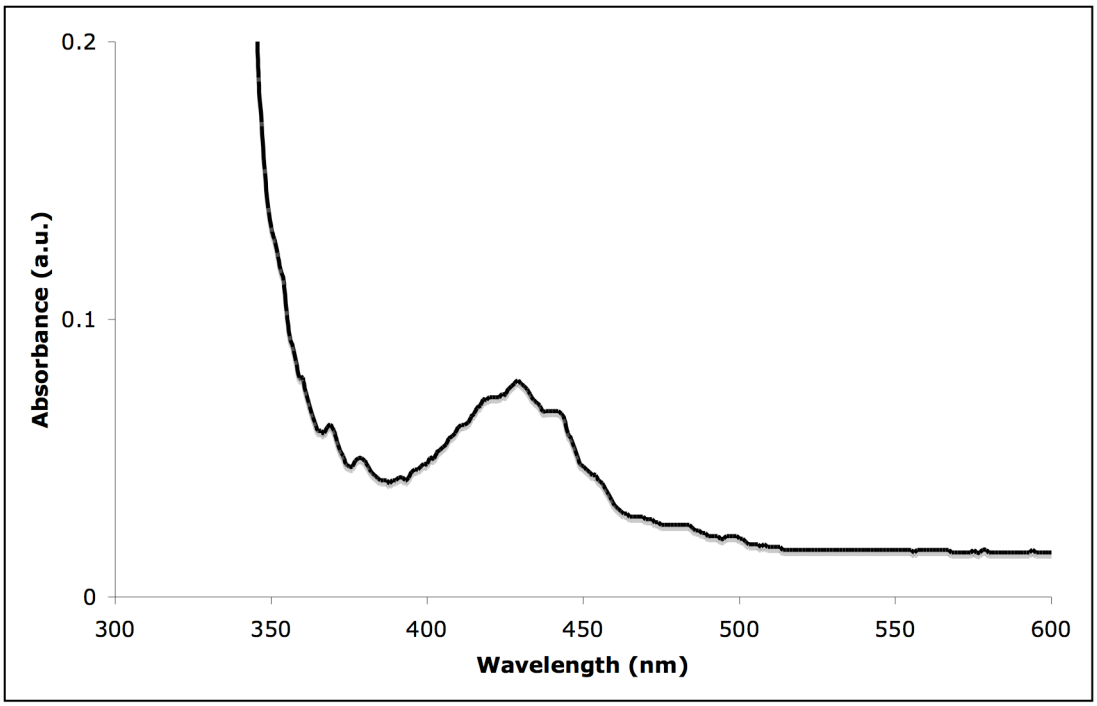

Figure S7. UV-vis spectrum of $[UO_2(TPIP)_2]_2$ (**6**) in CH_2Cl_2 (295 K)

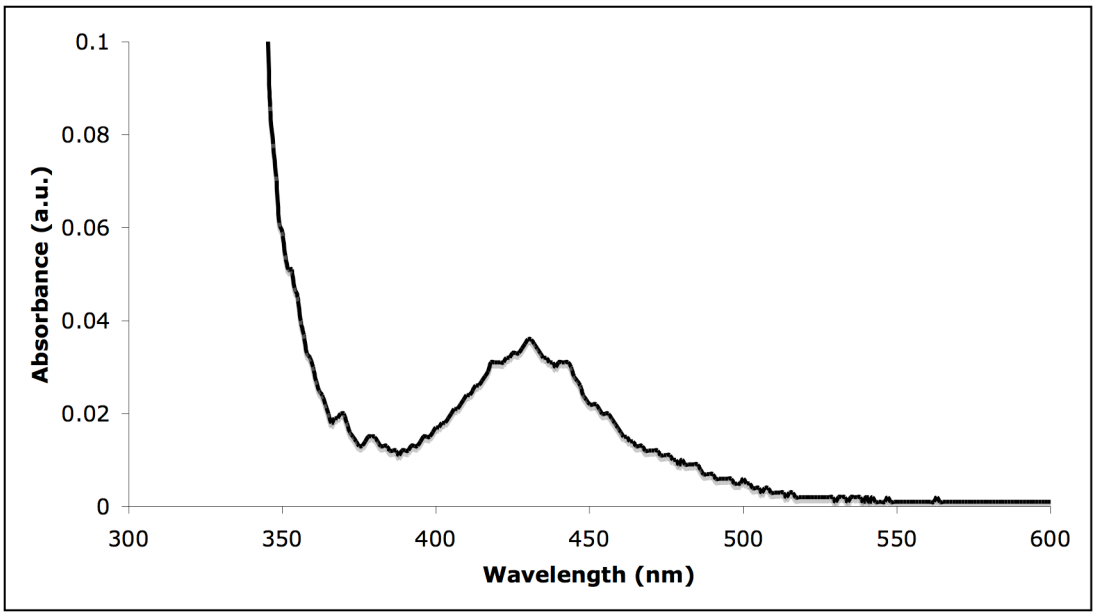

Figure S8. UV-vis spectrum of $[UO_2(TPIP)_2]_3$ (**7**) in CH_2Cl_2 (295 K)

Figure S9. VT (298–201 K) $^{31}P\{^{1}H\}$ NMR spectra of $[UO_2(TPIP)_2(THF)]$ **(4)** in CD_2Cl_2 (spectra offset).

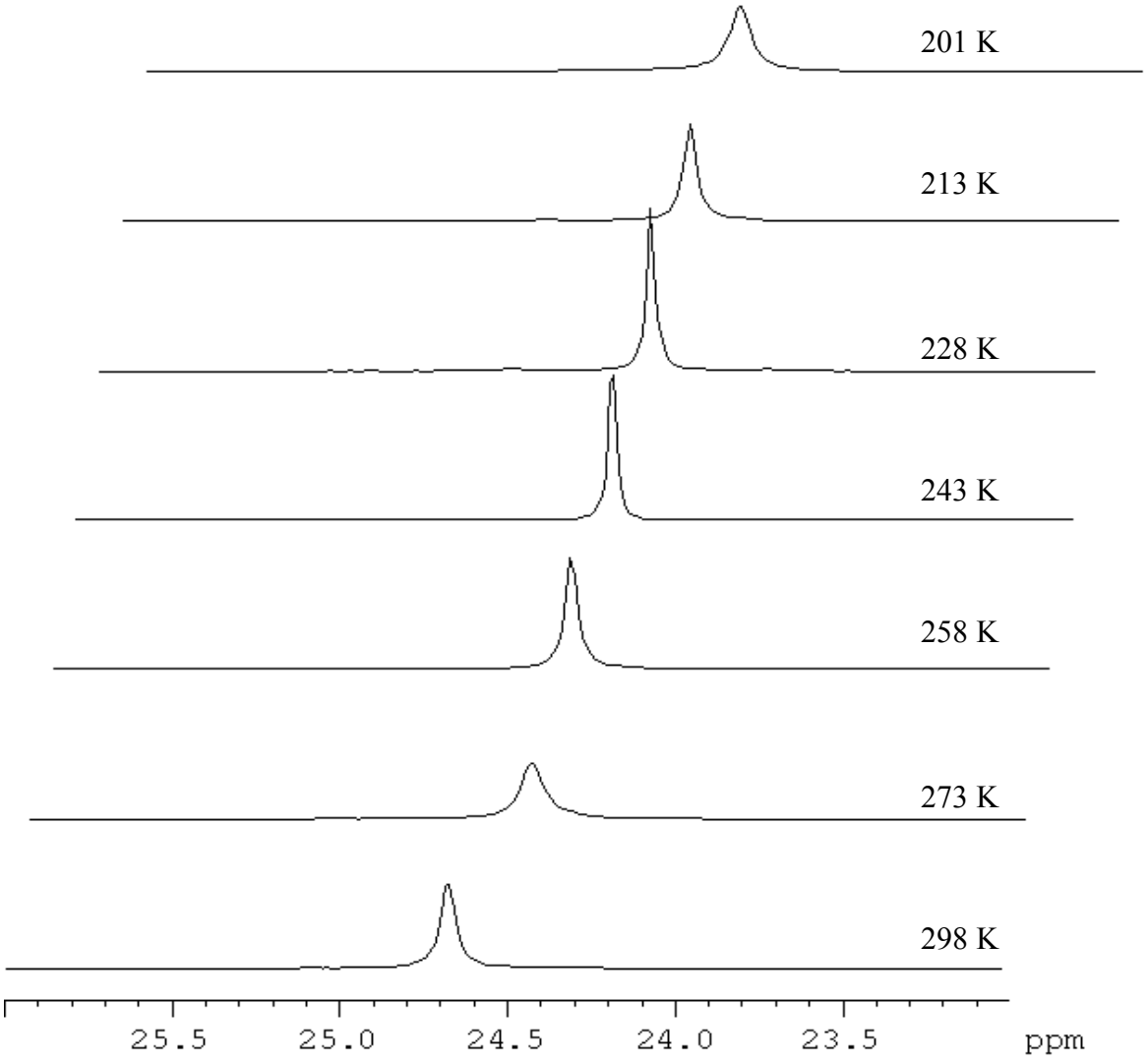

Figure S10. VT (298–213 K) ^{1}H NMR spectra of $[UO_2(TPIP)_2(OPCy_3)]$ **(5)** in CD_2Cl_2.

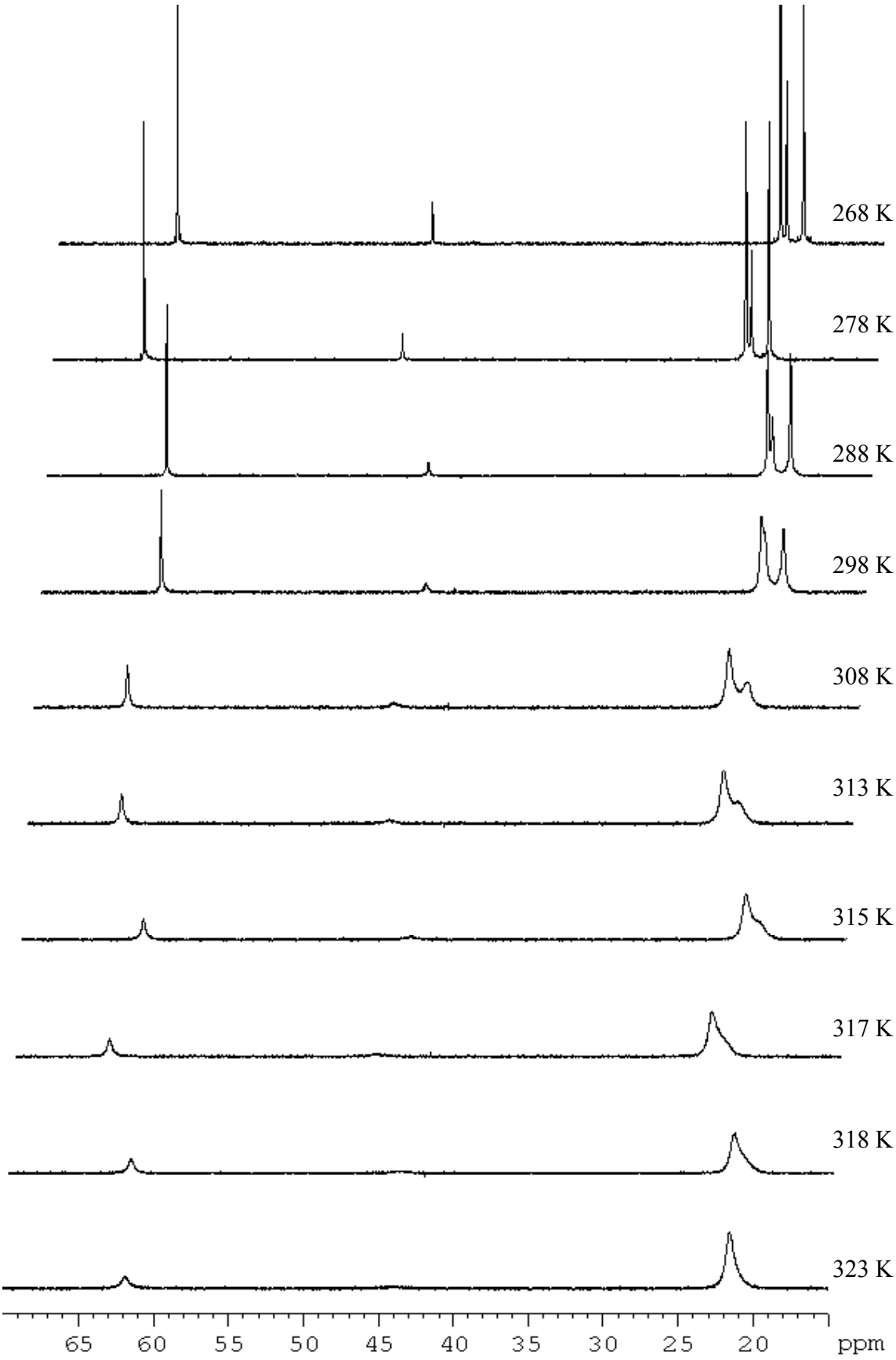

Figure S11. Thermal ellipsoid drawing of $[UO_2(TPIP)_2]_3$ (**7**) at the 50 % probability level; H atoms and lattice solvent molecules not shown.

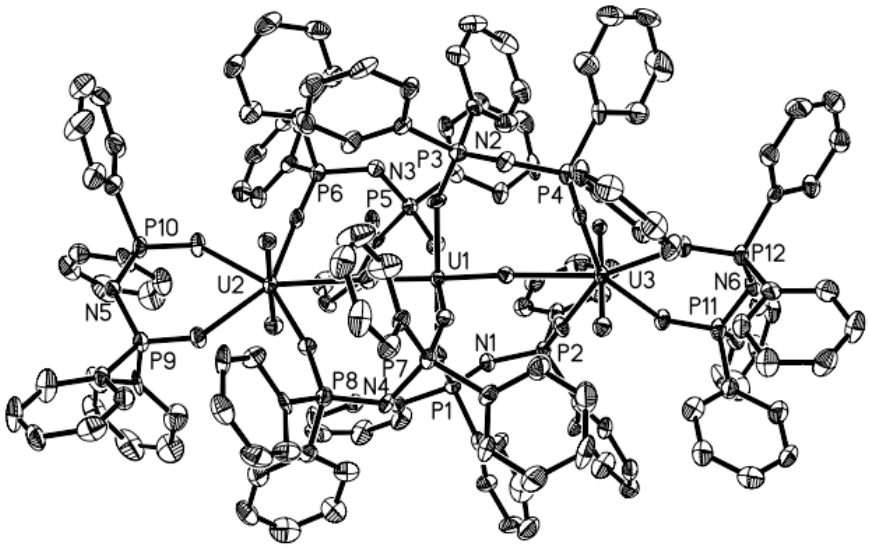

Table S1. Data collection and structural refinement for **7**

Complex	**7**.0.5C_6H_{14}
Empirical formula	C_{144} H_{120} N_6 O_{18} P_{12} U_3, 0.5(C_6 H_{14})
Formula weight	3351.28
Temperature (K)	100(2)
Wavelength (Å)	0.71073
Crystal system , space group	Monoclinic, $P2_1/c$
a, b, c (Å)	20.5618(15), 22.3000(16), 29.998(2)
α, β, γ (°).	90, 92.282(1), 90
Volume ($Å^3$))	13744.1(17)
Z	4
Density (calculated) (Mg/m^3)	1.620
Absorption coefficient (mm^{-1})	3.734
Crystal form, colour	Plate, yellow
Crystal size (mm^3)	0.20 x 0.20 x 0.05
Theta range for data collection (°)	2.08 to 25.03
Index ranges	-24<=h<=24, -26<=k<=26, -35<=l<=35
No. of measured, independent, observed reflections (I>2σ(*I*))	97209, 24254, 15597
R(int)	0.1161
Absorption correction	Semi-empirical from equivalents

$T_{max,}$ T_{min}	1.000, 0.668
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	24254 / 96 / 1676
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0506, 0.0805, 1.109
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.316, -1.359