

## Electronic supplementary information

**Table S-1.** Cartesian coordinates (Å) for UO<sub>2</sub>Cl<sub>2</sub>ac<sub>4</sub>.

	X	Y	Z
U	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.807187
O	0.000000	0.000000	-1.807187
Cl	2.721728	0.000000	0.000000
Cl	-2.721728	0.000000	0.000000
O	-1.167786	2.423003	0.453005
O	1.167786	-2.423003	0.453005
O	1.167786	2.423003	-0.453005
O	-1.167786	-2.423003	-0.453005
C	-1.841927	2.951108	1.341227
C	1.841927	-2.951108	1.341227
C	1.841927	2.951108	-1.341227
C	-1.841927	-2.951108	-1.341227
C	-2.349270	4.362327	1.153526
C	2.349270	-4.362327	1.153526
C	2.349270	4.362327	-1.153526
C	-2.349270	-4.362327	-1.153526
C	-2.238527	2.214312	2.589535
C	2.238527	-2.214312	2.589535
C	2.238527	2.214312	-2.589535
C	-2.238527	-2.214312	-2.589535
H	-3.451423	4.348349	1.128973
H	3.451423	-4.348349	1.128973
H	3.451423	4.348349	-1.128973
H	-3.451423	-4.348349	-1.128973
H	-2.061478	4.987676	2.012609
H	2.061478	-4.987676	2.012609
H	2.061478	4.987676	-2.012609

H	-2.061478	-4.987676	-2.012609
H	-1.965175	4.791124	0.221974
H	1.965175	-4.791124	0.221974
H	1.965175	4.791124	-0.221974
H	-1.965175	-4.791124	-0.221974
H	-2.975661	1.453990	2.276702
H	2.975661	-1.453990	2.276702
H	2.975661	1.453990	-2.276702
H	-2.975661	-1.453990	-2.276702
H	-1.381218	1.654645	2.984253
H	1.381218	-1.654645	2.984253
H	1.381218	1.654645	-2.984253
H	-1.381218	-1.654645	-2.984253
H	-2.676379	2.870754	3.351122
H	2.676379	-2.870754	3.351122
H	2.676379	2.870754	-3.351122
H	-2.676379	-2.870754	-3.351122

**Table S-2.** Cartesian coordinates (Å) for  $\text{UO}_2\text{Cl}_2\text{ac}_3$ .

	X	Y	Z
U	0.000000	0.000000	0.000000
O	1.799961	0.000000	0.000000
O	-1.794251	0.143254	0.000000
Cl	-0.031687	-0.795026	2.579869
Cl	-0.031687	-0.795026	-2.579869
O	-0.097284	-2.440833	0.000000
O	0.088048	2.209103	1.380037
O	0.088048	2.209103	-1.380037
C	-0.146350	-3.671898	0.000000
C	-0.176477	-4.427764	1.301978
C	-0.176477	-4.427764	-1.301978
C	0.117728	2.953765	2.362374

C	0.117728	2.953765	-2.362374
C	0.097381	2.443279	3.775354
C	0.097381	2.443279	-3.775354
C	0.177479	4.452903	2.159540
C	0.177479	4.452903	-2.159540
H	0.679609	-5.118945	1.349163
H	-1.084857	-5.048619	-1.349163
H	-1.084857	-5.048619	1.349163
H	0.679609	-5.118945	-1.349163
H	-0.148476	-3.725247	2.141680
H	-0.148476	-3.725247	-2.141680
H	0.994905	2.800991	4.304811
H	-0.768825	2.871288	-4.304811
H	-0.768825	2.871288	4.304811
H	0.994905	2.800991	-4.304811
H	0.053745	1.348464	3.784533
H	0.053745	1.348464	-3.784533
H	1.077749	4.861172	2.643801
H	-0.687442	4.931528	-2.643801
H	-0.687442	4.931528	2.643801
H	1.077749	4.861172	-2.643801
H	0.187074	4.693660	1.092596
H	0.187074	4.693660	-1.092596

**Table S-3.** Cartesian coordinates (Å) for [UO<sub>2</sub>Cl<sub>3</sub>ac<sub>2</sub>]<sup>-</sup>.

	X	Y	Z
U	0.000000	0.000000	0.000000
O	1.804559	0.000000	0.000000
O	-1.800841	0.115780	0.000000
Cl	0.090667	2.823374	0.000000
Cl	-0.066929	-2.084195	1.766731
Cl	-0.066929	-2.084195	-1.766731

O	0.029753	0.926510	2.386863
O	0.029753	0.926510	-2.386863
C	0.041817	1.302184	3.550293
C	0.041817	1.302184	-3.550293
C	0.089317	2.781347	3.866306
C	0.089317	2.781347	-3.866306
C	0.009644	0.300340	4.682163
C	0.009644	0.300340	-4.682163
H	0.107397	3.344352	2.925348
H	0.107397	3.344352	-2.925348
H	0.981853	3.009416	4.470704
H	-0.786746	3.066211	-4.470704
H	-0.786746	3.066211	4.470704
H	0.981853	3.009416	-4.470704
H	-0.022885	-0.712660	4.262222
H	-0.022885	-0.712660	-4.262222
H	0.898828	0.426842	5.320601
H	-0.869590	0.483631	-5.320601
H	-0.869590	0.483631	5.320601
H	0.898828	0.426842	-5.320601

**Table S-4.** Cartesian coordinates (Å) for [UO<sub>2</sub>Cl<sub>3</sub>ac]<sup>-</sup>.

	X	Y	Z
U	0.000000	0.000000	0.000000
O	1.810037	0.000000	0.000000
O	-1.798148	0.207117	0.000000
Cl	-0.151024	-2.630992	0.000000
Cl	0.022991	0.400532	2.660622
Cl	0.022991	0.400532	-2.660622
O	0.143192	2.494548	0.000000
C	0.213452	3.718555	0.000000
C	0.256995	4.477119	1.304174

C	0.256995	4.477119	-1.304174
H	1.177251	5.079853	1.357025
H	-0.588246	5.181196	-1.357025
H	-0.588246	5.181196	1.357025
H	1.177251	5.079853	-1.357025
H	0.216434	3.770497	2.140118
H	0.216434	3.770497	-2.140118