Electronic Supporting Information

Combining coordination and supramolecular chemistry for the formation of uranyl-organic hybrid materials

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Synthesis of 1-3

Caution: Whereas the uranium nitrate hexahydrate ($UO_2(NO_3)_2{\cdot}6H_2O$) used in this study consists of depleted U, standard precautions for handling radioactive and toxic substances should be followed. All organics were purchased from Acros Organics and used without any further purification.

[$UO_2(ClC_6H_4COO)_2(H_2O)$] (1)

Compound **1**, was synthesized hydrothermally by combining $UO_2(NO_3)_2{\cdot}6H_2O$ (0.125 g, 250 μmol), 4-chlorobenzoic acid (0.074 g, 470 μmol), ammonium hydroxide (25μL), and distilled water (3.00 g, 0.167 mol) in a Teflon-lined, 23 mL stainless steel Parr bomb. The initial pH of the solution was 3.4. The Parr bomb was sealed, heated statically at 150 °C for 2 days and then cooled to room temperature. Two products, a white/tan powder and a yellow crystalline solid, were obtained. Separation of the yellow crystals from the white/tan phase was achieved through subsequent washing with ethanol and water. We note here the same reaction product is created without the addition of ammonium hydroxide (initial pH is 1.2), but the yield after two days is greatly reduced.

[$UO_2(BrC_6H_4COO)_2(H_2O)$] (2)

Compound **2**, was synthesized hydrothermally by combining $UO_2(NO_3)_2{\cdot}6H_2O$ (0.132 g, 262 μmol), 4-bromobenzoic acid (4Br-BA) (0.113 g, 560 μmol), ammonium hydroxide (25μL), and distilled water (3.00 g, 0.167 mol) in a Teflon-lined, 23 mL stainless steel Parr bomb. The initial pH of the solution was 3.0. The Parr bomb was sealed, heated statically at 150 °C for 2 days and then cooled to room temperature. Two products, a white/tan powder and a yellow crystalline solid, were obtained. Separation of the yellow crystals from the white/tan phase was achieved through subsequent washing with ethanol and water. We note here the same reaction product is created without the addition of ammonium hydroxide (initial pH is 1.4), but the yield after two days is greatly reduced.

[$UO_2(IC_6H_4COO)_2(H_2O)$] (3)

Compound **3**, was synthesized hydrothermally by combining $UO_2(NO_3)_2{\cdot}6H_2O$ (0.126 g, 250 μmol), 4-iodobenzoic acid (4I-BA) (0.126 g, 510 μmol), ammonium hydroxide (25μL), and distilled water (3.00 g, 0.167 mol) in a Teflon-lined, 23 mL stainless steel Parr bomb. The initial pH of the solution was 2.6. The Parr bomb was sealed, heated statically at 150 °C for 2 days and then cooled to room temperature. Two products, a white/tan powder and a yellow crystalline solid, were obtained. Separation of the yellow crystals from the white/tan phase was achieved through subsequent washing with ethanol and water. We note here the same reaction product is created without the addition of ammonium hydroxide (initial pH is 1.6), but the yield after two days is greatly reduced.

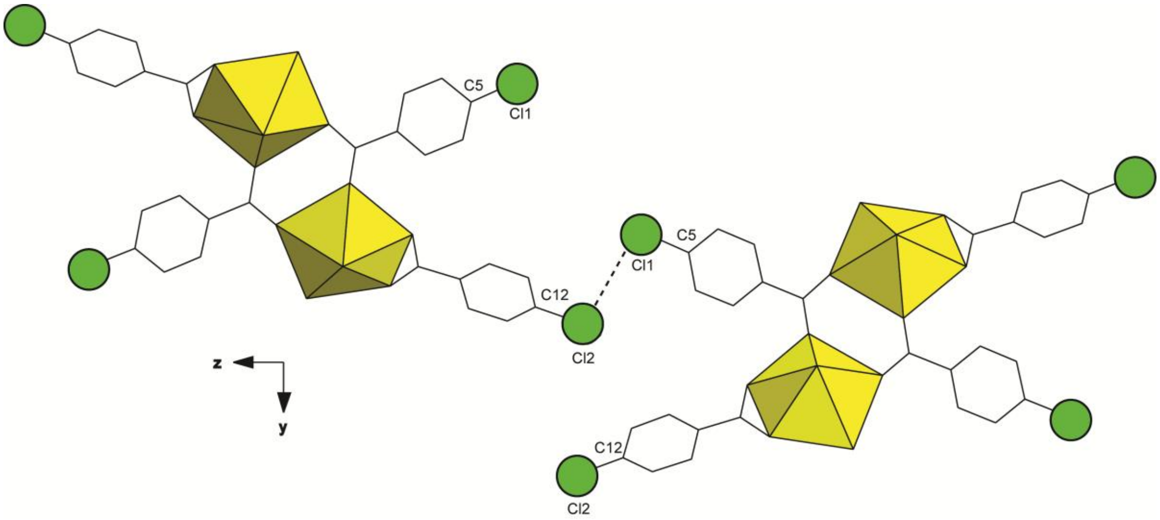

Fig.1 Polyhedral representation of the local structure of 1 showing Cl···Cl interaction described in Scheme 1 and packing along [1 0 0]. The uranium atoms are represented by the yellow polyhedra and the chlorides are shown in green. Hydrogen atoms have been omitted for clarity.

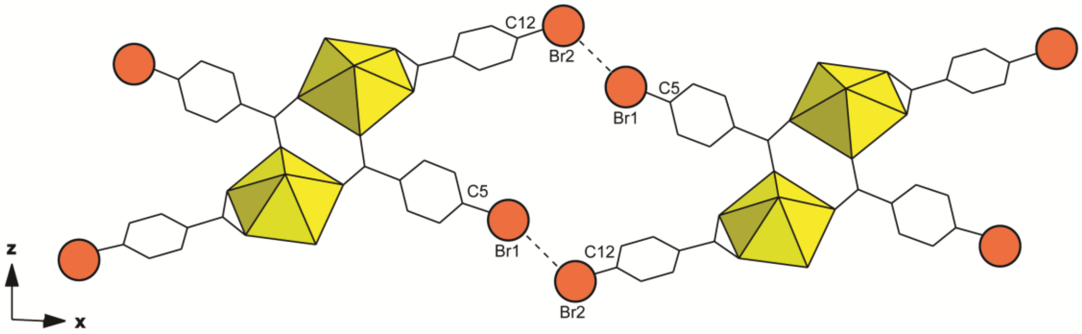

Fig.2 Polyhedral representation of the local structure of 2 (isostructural with 3) showing Br···Br interaction described in Scheme 1 and packing along [0 1 0].

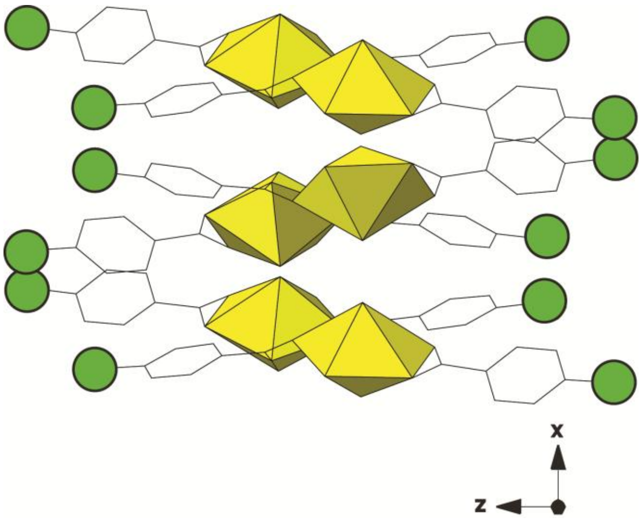

Fig S1. Polyhedral representation of the packing of 1 shown down the [0 1 0].

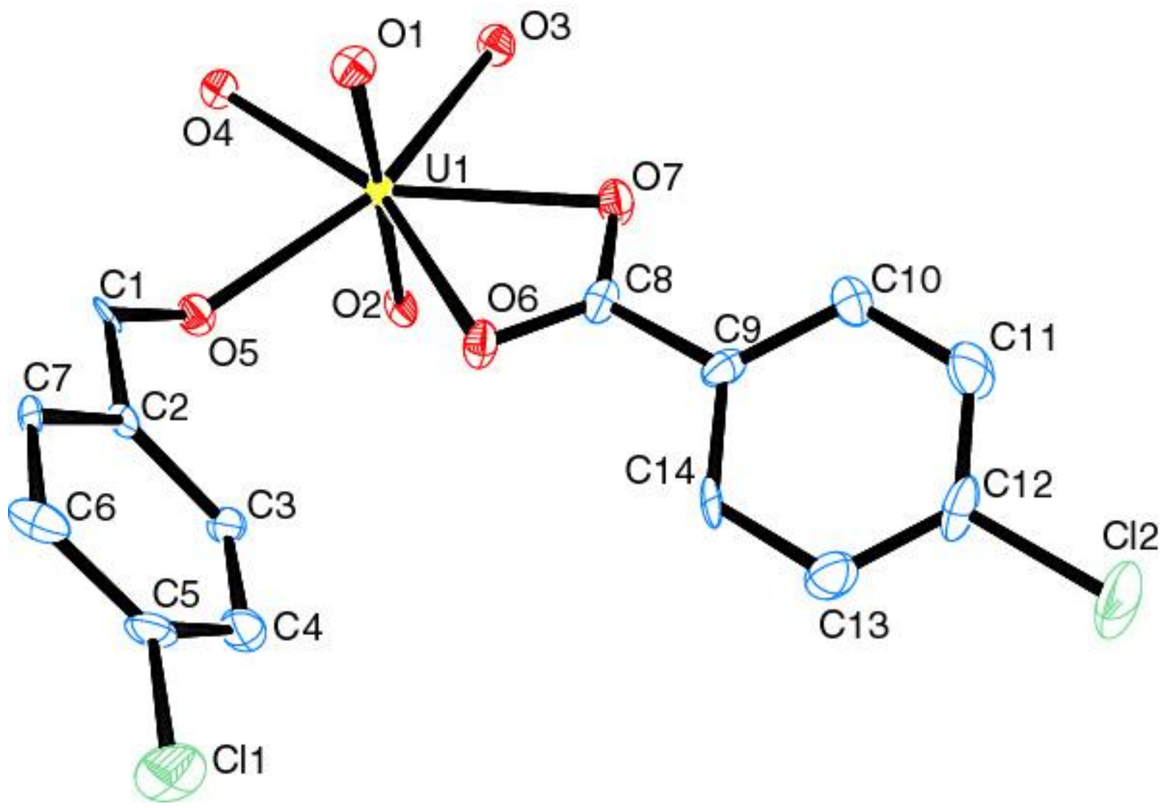

Fig S2. ORTEP illustration of **1**. Ellipsoids are shown at 50% probability level.

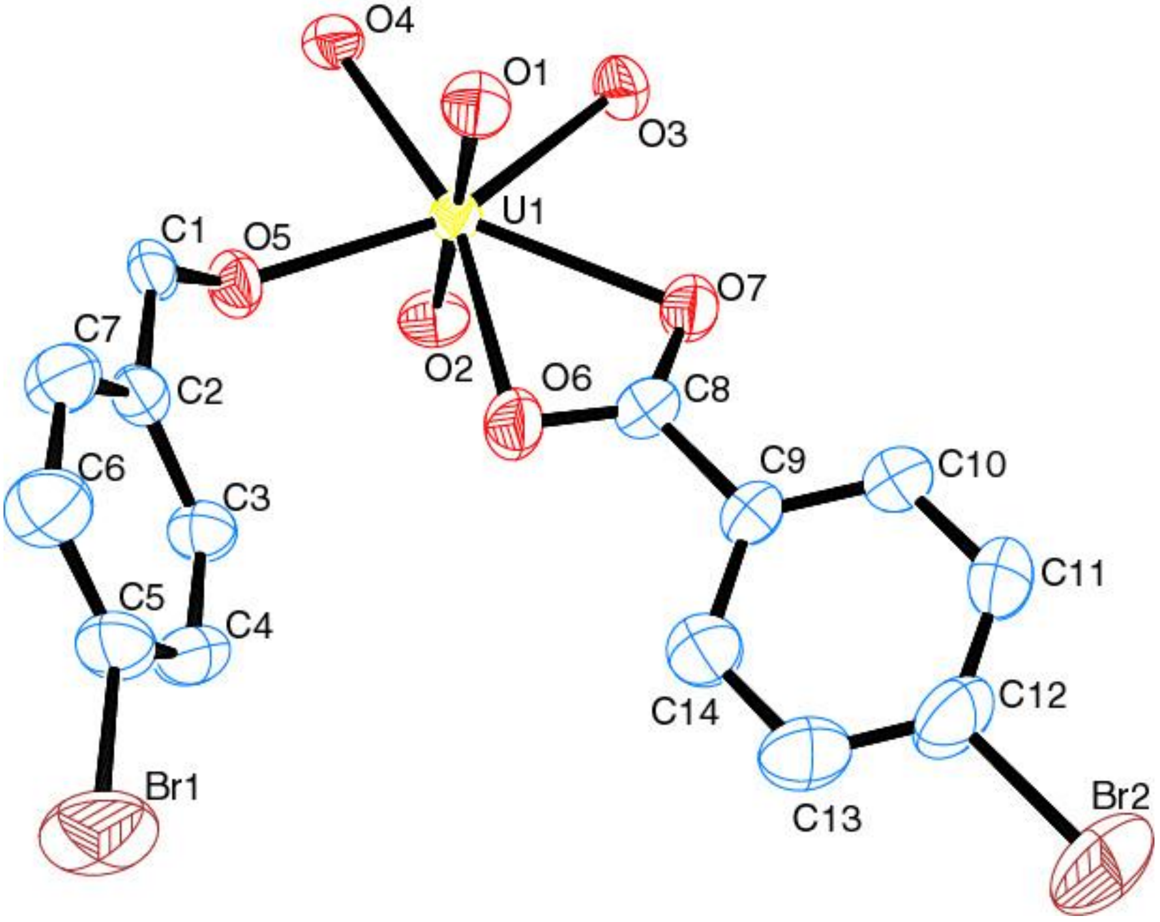

Fig S3. ORTEP illustration of **2**. Ellipsoids are shown at 50% probability level.

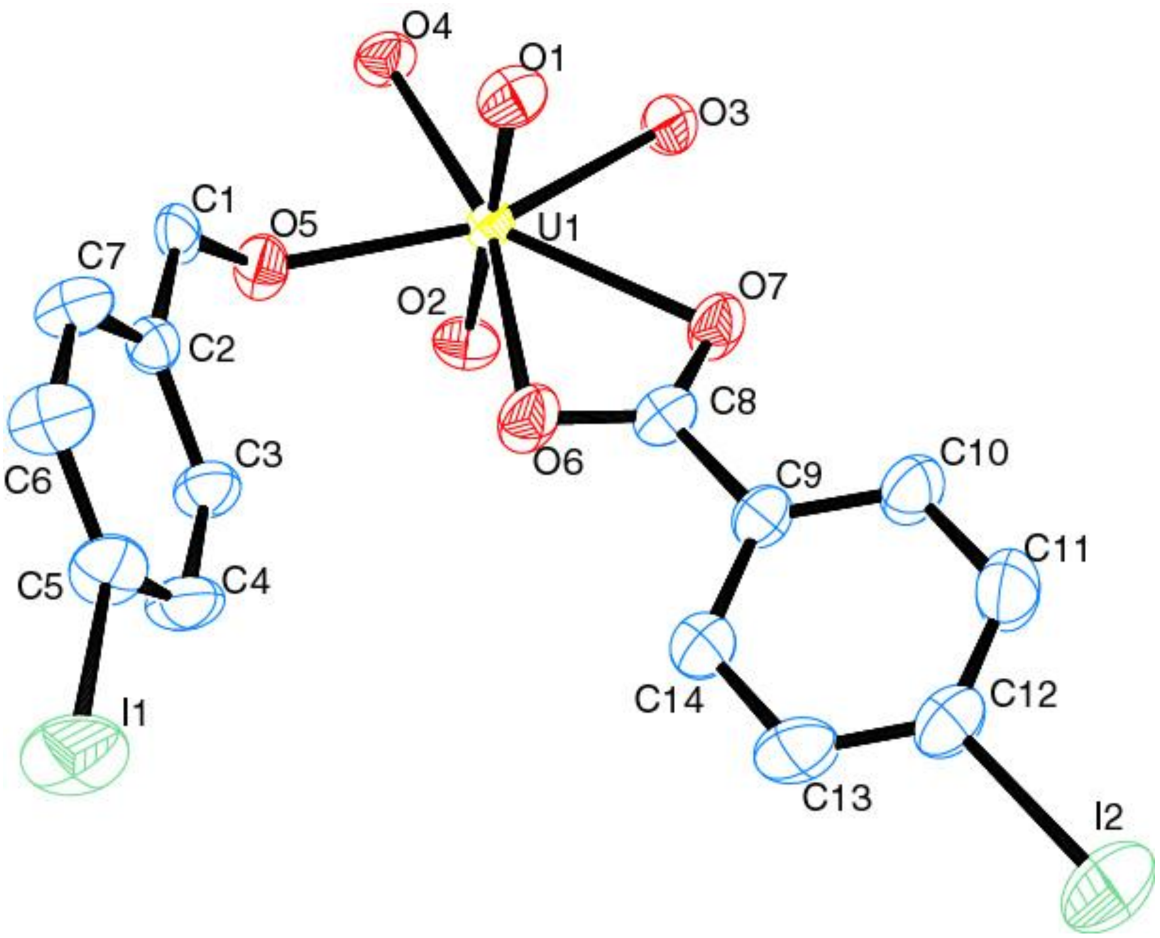

Fig S4. ORTEP illustration of **3**. Ellipsoids are shown at 50% probability level.

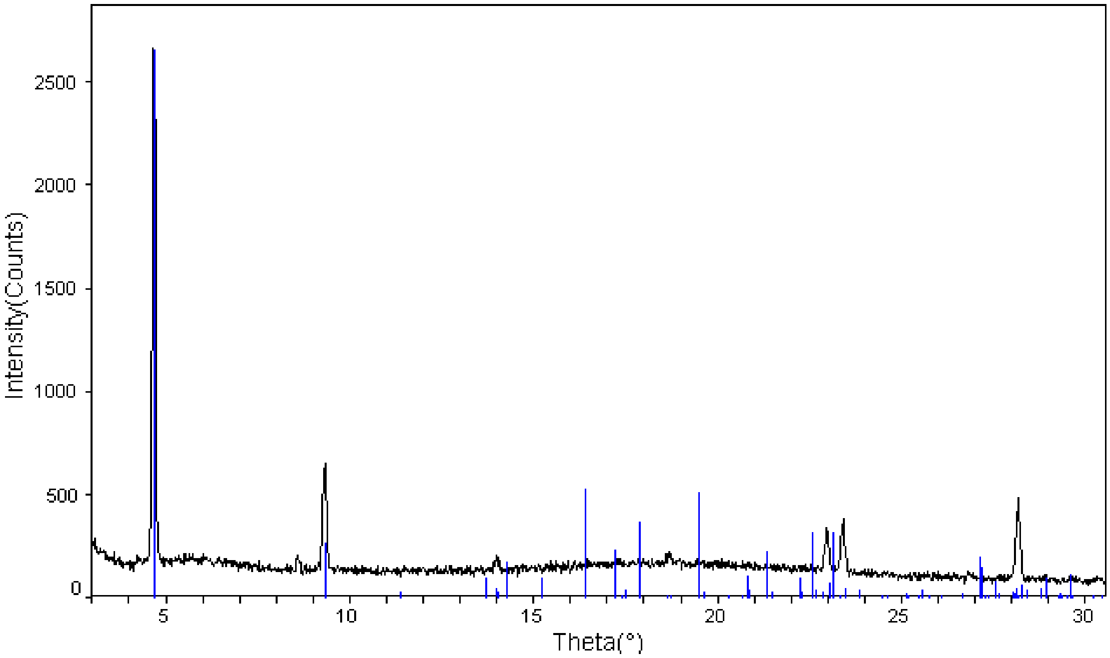

Fig S5. PXRD of **1** with calculated pattern overlaid in blue.

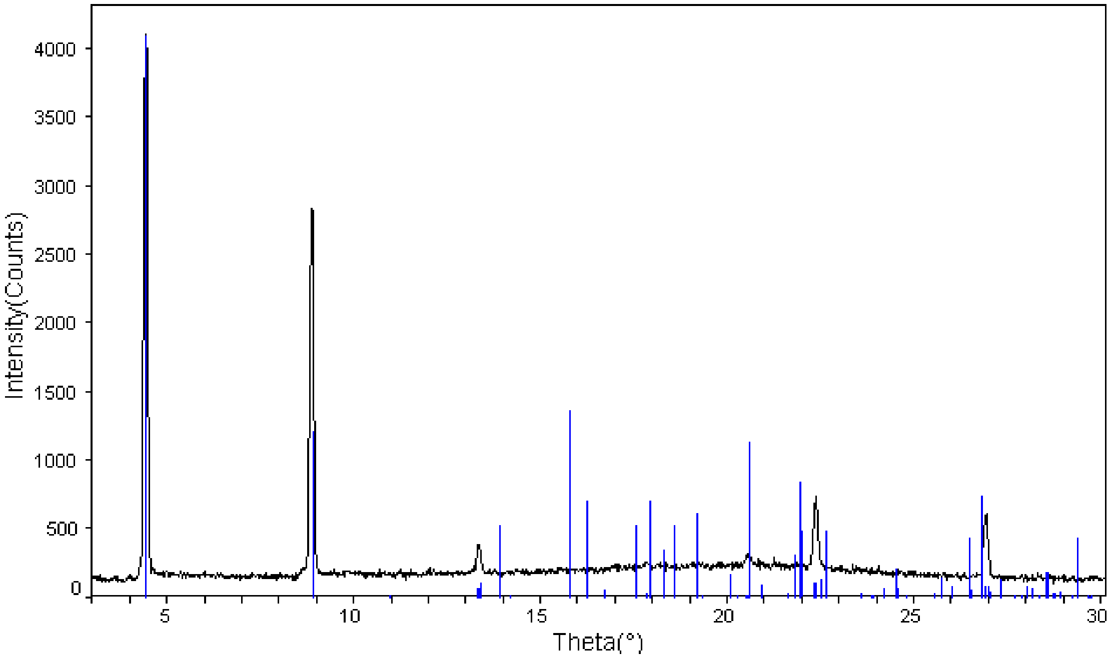

Fig S6. PXRD of **2** with calculated pattern overlaid in blue.

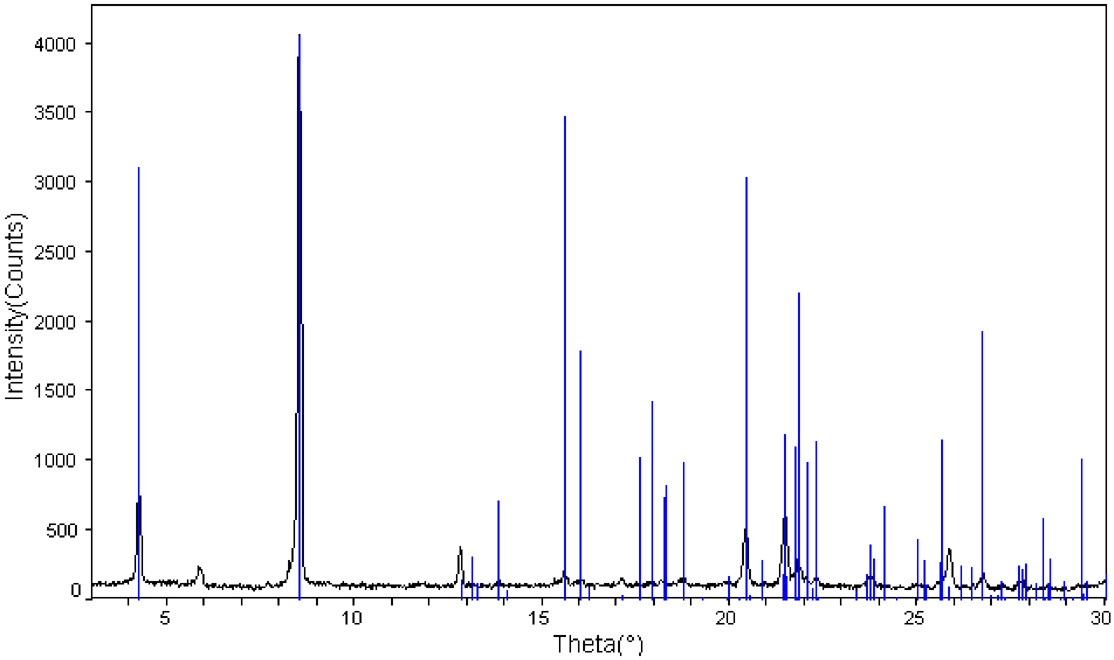

Fig S7. PXRD of **3** with calculated pattern overlaid in blue. We acknowledge a small impurity.

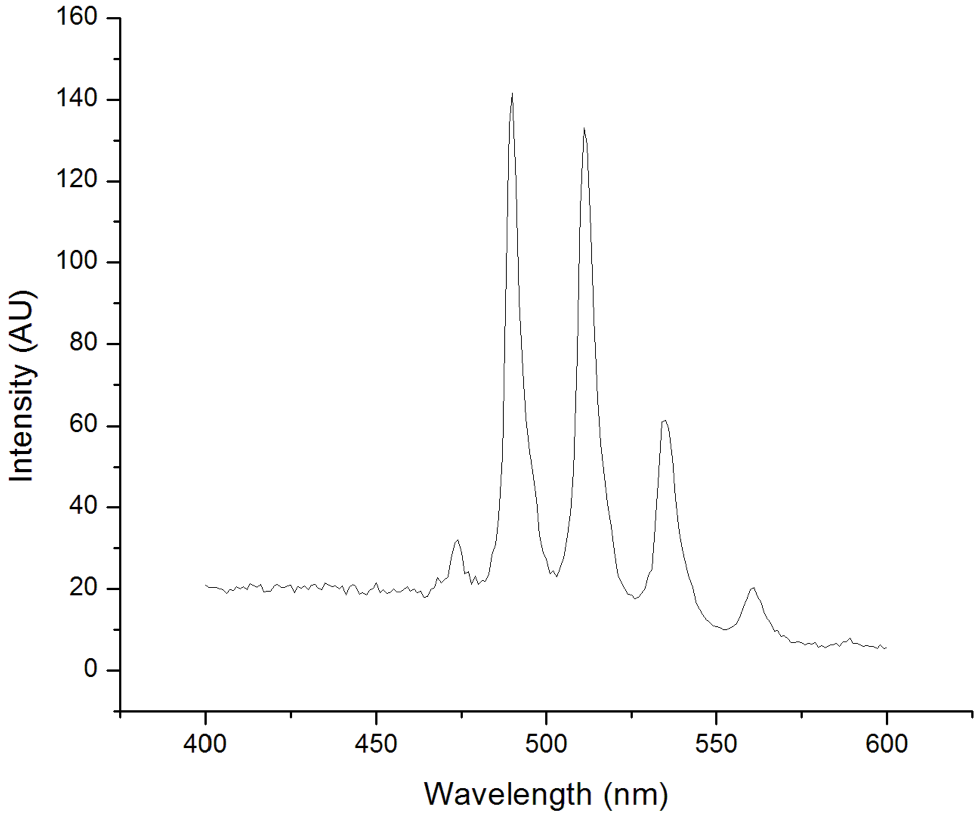

Fig S8. Emission spectra for compound **1** via uranyl excitation at 365 nm.

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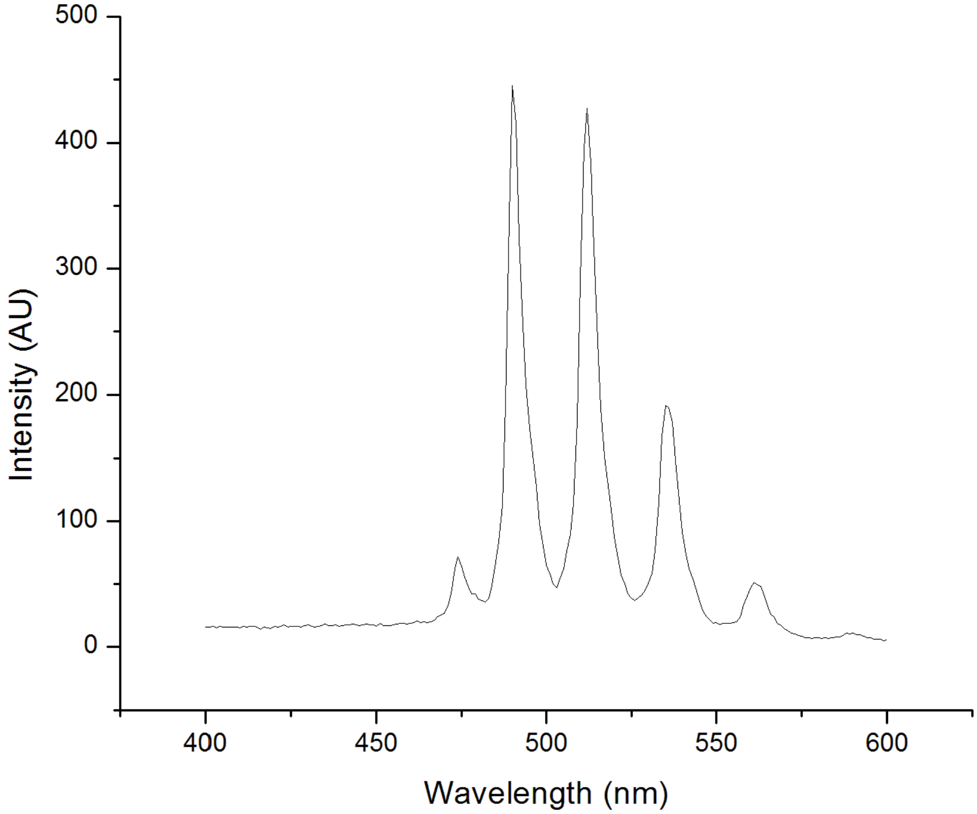

Fig S9. Emission spectra for compound **2** via uranyl excitation at 365 nm.

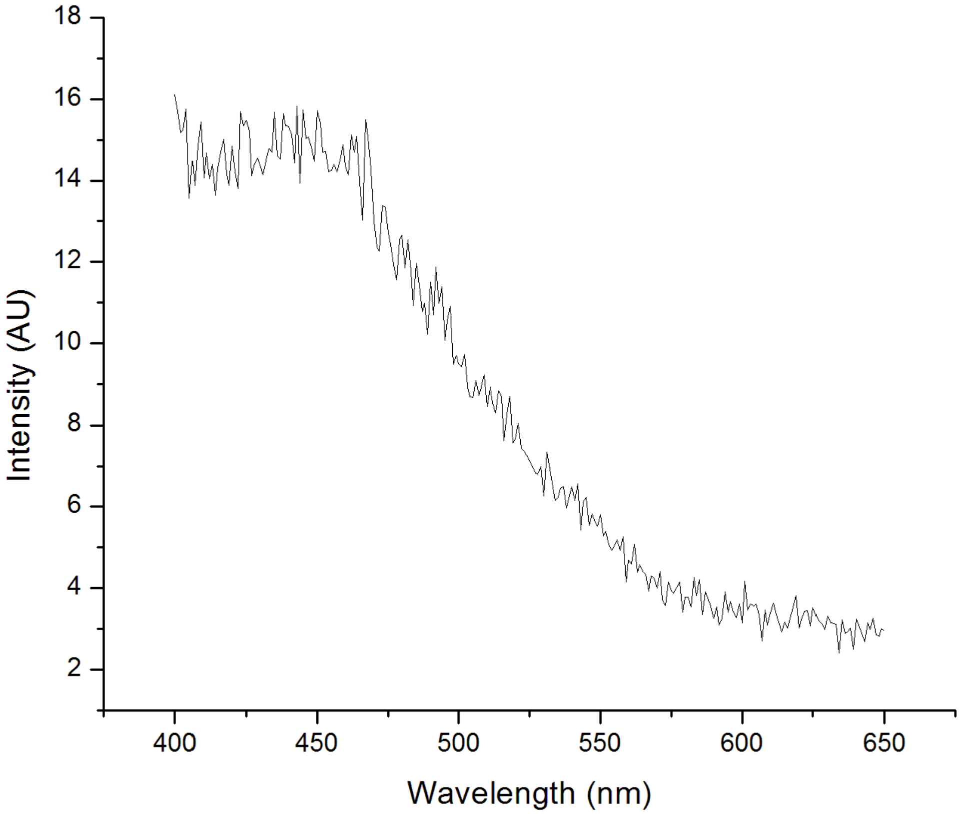

Fig S10. Emission spectra for compound **3** via uranyl excitation at 365 nm.