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Supporting information for article:

Utilizing bifurcated halogen-bonding interactions with the uranyl oxo group in the assembly of a UO2–3-bromo-5-iodobenzoic acid coordination polymer

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Supporting Info Section

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I. Additional Figures

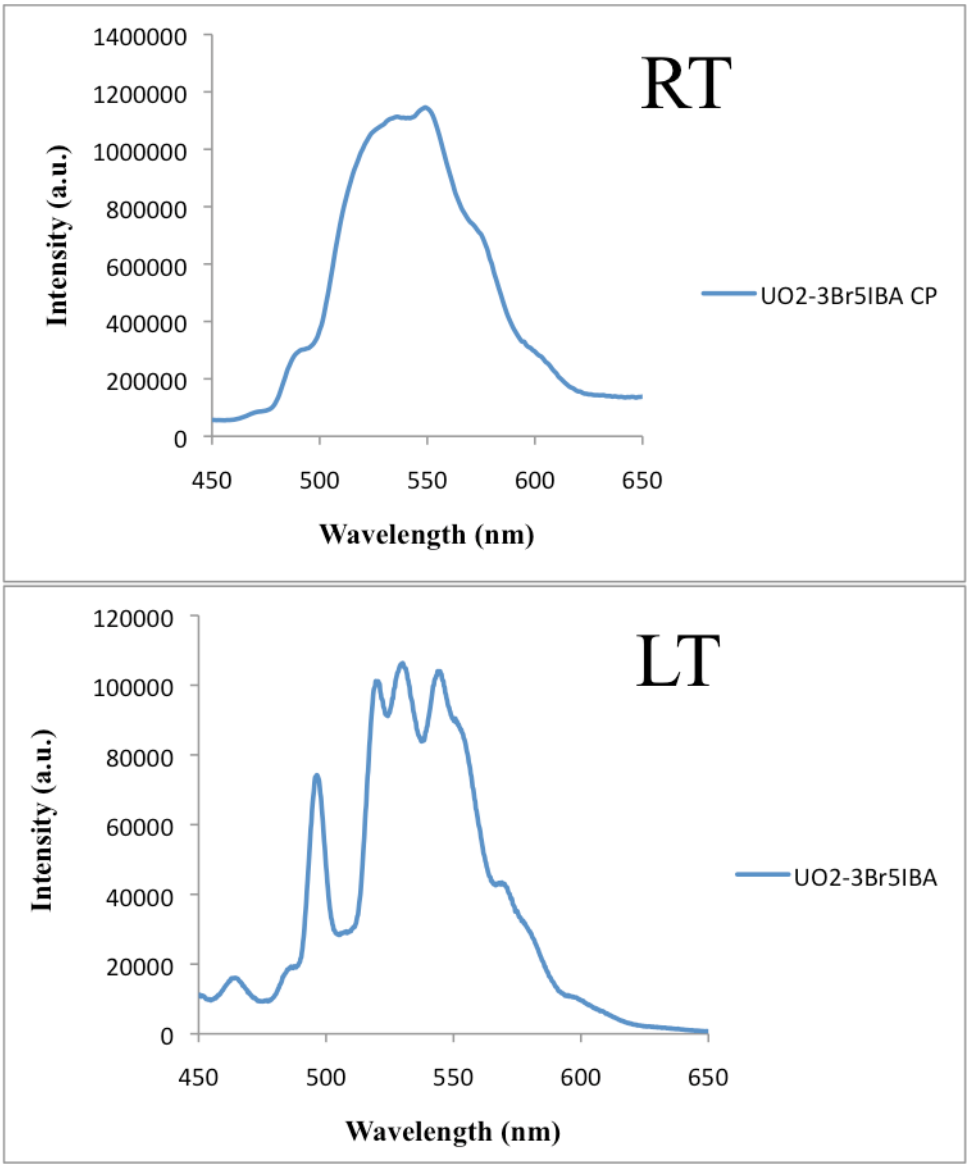

Figure S1 **(Top)** Room temperature, solid-state emission spectrum of **1**. **(Bottom**) Solid-state emission spectrum of **1** at 77K (LT).

II. Powder X-ray diffraction data

Table S1 Synthesis conditions to yield pure bulk product of **1**

Com-pound	Uranyl Nitrate (mols)	3Br5IBA (mols)	H_2O (mols)	Temperature (ºC)	Duration (hours)	5M NaOH (mols)
1	1	2.5	667	150	24	5

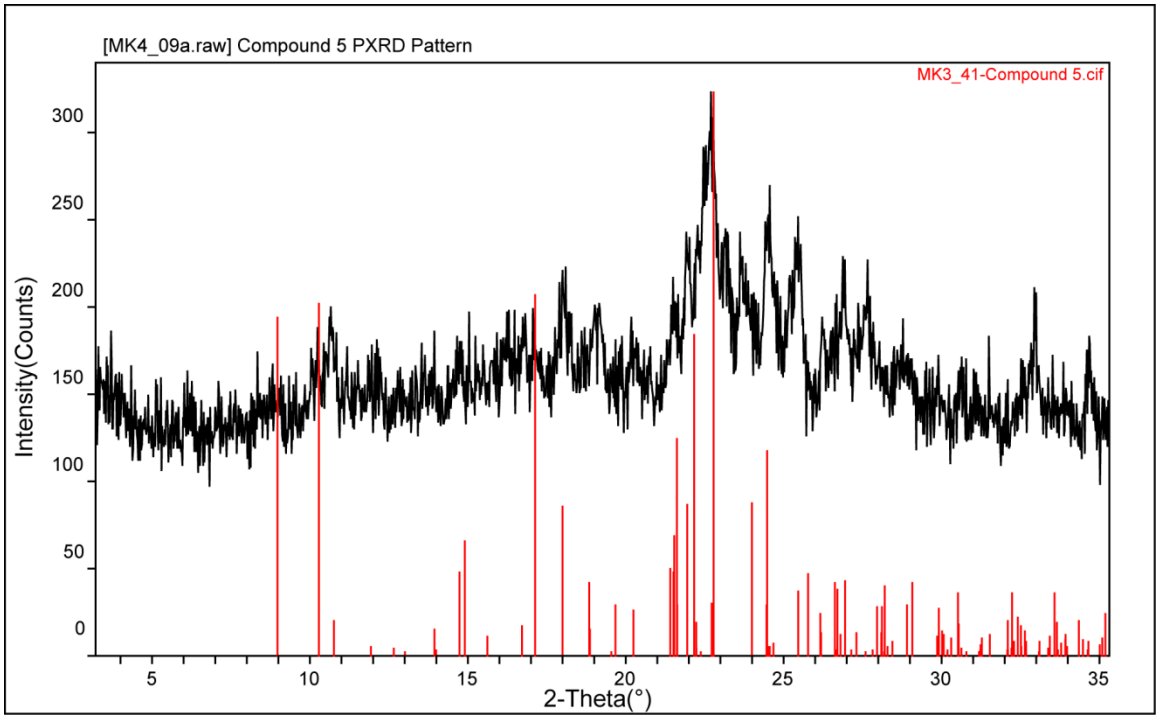

Figure S2 The observed PXRD pattern of structure **1** with calculated pattern overlaid in red.

III. Thermal Ellipsoid Plot

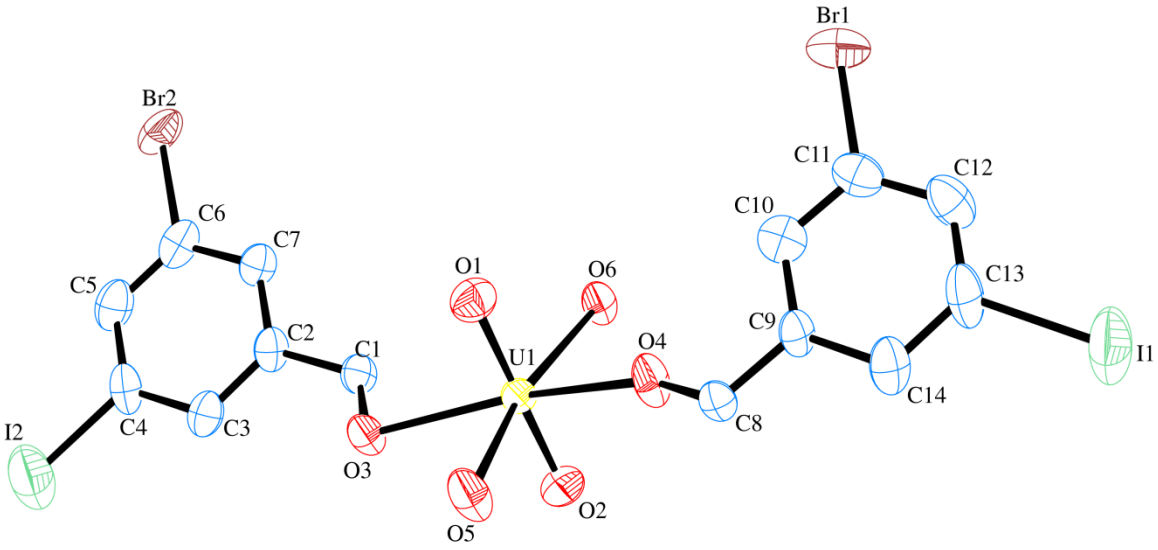

Figure S3 ORTEP illustration of compound **1**. Ellipsoids are shown at 50% probability level.

IV. Tables of Bond Distances

Table S2 Selected bond lengths and angles (Å, º) for the U(VI) coordination environment in compound **1**

Compound 1	**Distances [Å] and Angles [º]**
U1-O1	1.750(8)
U1-O2	1.759(9)
U1-O3	2.584(7)
U1-O4	2.438(7)
U1-O5	2.295(7)
U1-O6	2.294(8)
U1-O6’	2.414(7)

O1-U1-O2	178.2(4)
O1-U1-O3	82.9(3)
O1-U1-O4	88.0(3)
O1-U1-O5	87.9(4)
O1-U1-O6	90.5(4)
O1-U1-O6’	92.3(3)
O2-U1-O3	95.6(3)
O2-U1-O4	91.7(3)
O2-U1-O5	93.0(4)
O2-U1-O6	91.1(4)
O2-U1-O6’	86.3(3)
O3-U1-O4	146.5(2)
O3-U1-O5	65.4(3)
O3-U1-O6	51.6(2)
O3-U1-O6’	116.4(2)
O4-U1-O5	76.8(3)
O4-U1-O6	128.0(2)
O4-U1-O6’	84.0(3)
O5-U1-O6	160.3(3)
O5-U1-O6’	166.6(3)
O6-U1-O6’	83.0(3)

Symmetry code to generate equivalent atoms: -x+2, -y+1, -z+1

V. Actinyl Force Constants

Table S3 Symmetric (υ_1) and asymmetric (υ_1) stretches for compound **1** along with stretching force (k_1, mdyn/Å) and interaction force (k_{12}, mdyn/Å) constants for the O=An=O bond.

Complex	**υ_1 (cm^{-1})**	**υ_3 (cm^{-1})**	**k_1 (mdyn/Å)**	**k_{12} (mdyn/Å)**	**Supra-molecular Int.**	**Sum of vdW (%)**
UO_2^{2+} (aq)	860-880	930-960				
$[UO_2(C_7H_3BrIO_2)_2]_n$ **(1)**	854	946	7.15	-0.28	I-oxo Br-oxo	92.8, 97.5