Structural, Spectroscopic, and Computational Evaluations of Cation-Cation and Halogen Bonding Interactions in Heterometallic Uranyl Hybrid Materials

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Supporting Info Section

I. Additional Figures and Tables

Table S1 Crystallographic Data for **1-4**

	1	**2**	**3**	**4**
chem formula	$C_{28}H_{16}I_4N_2O_{18}Ag_2U_2$	$C_{21}H_{12}I_3O_8AgU$	$C_{21}H_{12}I_3O_8AgU$	$C_{21}H_9I_6O_8AgU$
formula weight	1867.83	1118.91	1118.91	1496.58
crystal system	triclinic	triclinic	monoclinic	triclinic
space group	P-1	P-1	$P2_1/n$	P-1
a (Å)	8.8109(4)	8.677(7)	9.1545(5)	11.210(7)
b (Å)	11.4713(6)	9.815(8)	14.2946(7)	12.407(8)
c (Å)	11.4852(6)	15.0560(11)	19.4243(10)	23.0870(11)
α (deg)	117.072(4)	97.859(6)	90	77.655(6)
β (deg)	106.043(3)	98.971(7)	93.878(11)	82.316(6)
γ (deg)	91.445(3)	101.625(7)	90	74.954(7)
V (Å^3)	977.81(9)	1221.7(14)	2536.0(2)	3019.0(3)
Z	1	2	4	4
T (K)	293(2)	293(2)	293(2)	293(2)
λ (Mo Kα)	0.71073	0.71073	0.71073	0.71073
D_{calc} (g cm^{-3})	3.172	3.042	2.931	3.293
μ (mm^{-1})	12.476	11.256	10.845	12.183
R_{int}	0.0297	0.0662	0.0421	0.0332
R1 [$I>2\sigma(I)$]	0.0384	0.0419	0.0297	0.0387
wR2 [$I>2\sigma(I)$]	0.0879	0.0821	0.0720	0.0849
CCDC Number	2038396	2038397	2038398	2038399

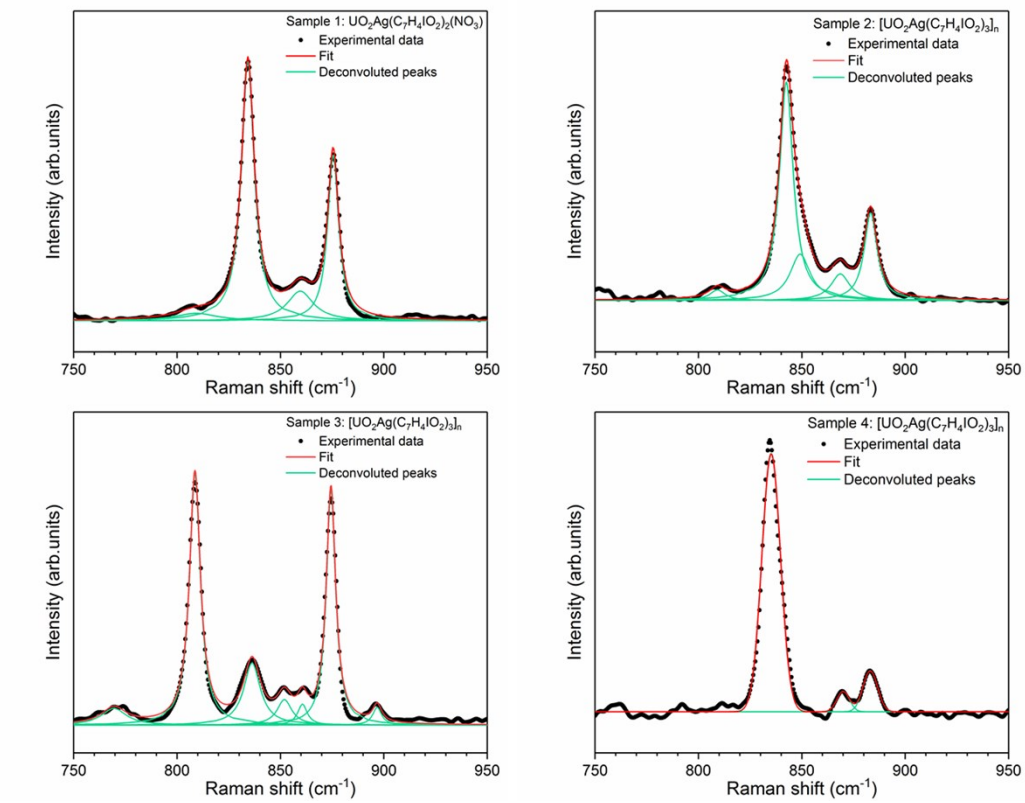

Figure S1 Deconvolution of Raman spectra of **1-4** for peak identification using Lorentzian curves.[1, 2] From these peak deconvolutions, we were able to extract Raman frequencies and vibrational peak modes, which are highlighted in Figure 9.

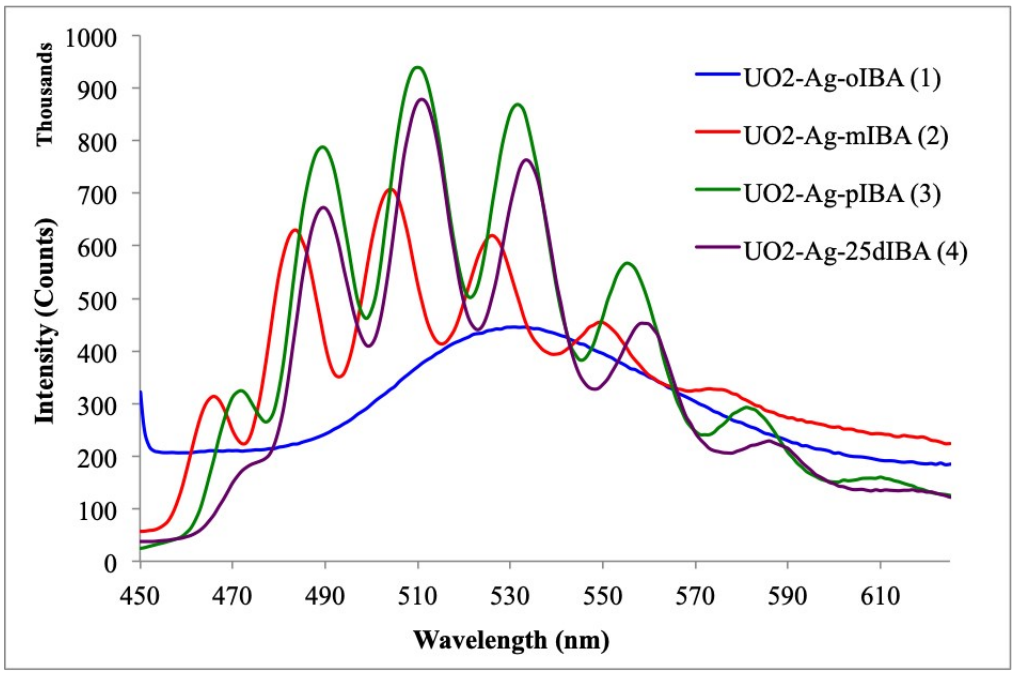

Figure S2 Room temperature, solid-state emission spectra of **1-4**.

Table S2 Summary of peak positions and vibronic gaps of solid-state emission spectra of **1-4**.

Compound	Peak Positions from Emission Spectra (nm)	Vibronic Gaps between Emission Spectra Peaks (cm^{-1})	Average Vibronic Gap (cm^{-1})
1	n/a	n/a	n/a
2	466, 484, 504, 526, 550, 575	792, 842, 830, 811, 805	816
3	472, 489, 509, 532, 556, 582, 610	761, 813, 827, 805, 819, 798	804
4	474, 490, 510, 559, 587, 620	830, 865, 837, 840, 906	856

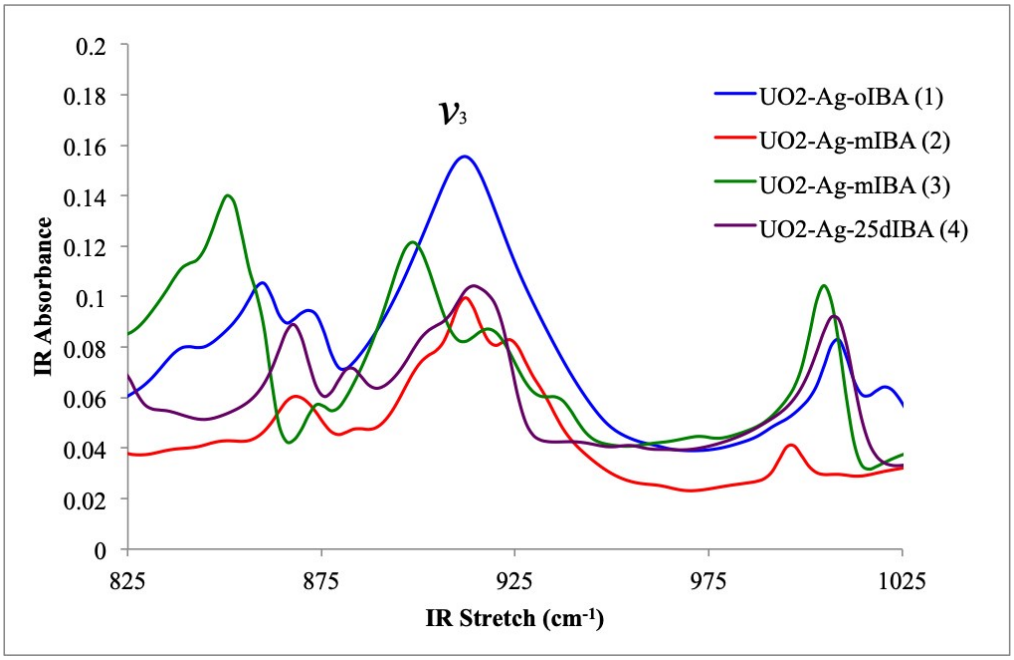

Figure S3 IR spectra of **1-4**. Asymmetric stretch (ν_3) of the uranyl cation is highlighted for each complex.

Table S3 U-O Axial Bond Lengths in **1-4**.

Compound	d_{U1-O1} [Å]	d_{U1-O2} [Å]	d_{U2-O3} [Å]	d_{U2-O4} [Å]
1	1.746(7)	1.743(7)		
2	1.746(6)	1.768(6)		
3	1.772(4)	1.793(4)		
4	1.747(6)	1.777(5)	1.776(5)	1.750(6)

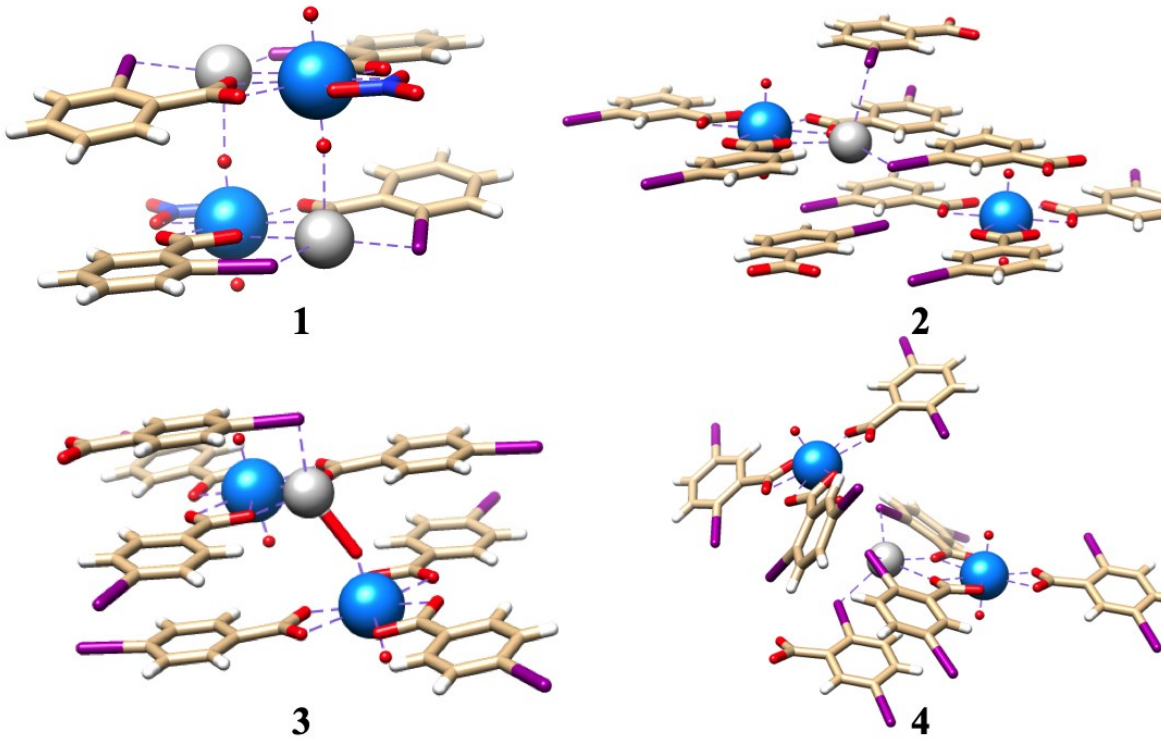

Figure S4 Model structures of **1-4**. Ball and stick representation is indicative of those atoms whose positions were optimized or partially optimized.

Table S4 Comparison of experimental and DFT calculated values of (ν_1) for **1-4**.

Compound	ν (cm^{-1})	Expt.	Notes
1	853	834.5	Uranyl 1 has greater amplitude
1	857		Uranyl 2 has greater amplitude
2	843	842.5	Localized on uranyl 1
2	855		Localized on uranyl 2 (I coordination, Ag in 2nd sphere)
3	765	808.5	Localized on uranyl 1 (Ag coordinating uranyl O)
3	796		Localized on uranyl 2
4	837	834.5	Localized on uranyl 1 (2 x I coordination)
4	850		Localized on uranyl 2 (Ag in 2nd coordination sphere)

Table S5 Comparison of experimental and DFT calculated values of (ν_3) for **1-4**.

Compound	ν (cm^{-1})	Expt.	Notes
1	916	912	Uranyl 2 has greater amplitude
1	920		Uranyl 1 has greater amplitude
2	899	912	Localized on uranyl 1
2	909		Localized on uranyl 2 (I coordination, Ag in 2nd sphere)
3	826		Localized on uranyl 1 (Ag coordinating uranyl O)
3	860	898	Localized on uranyl 2 (coupled to equatorial vibrations)
3	866		Localized on uranyl 2 (coupled to equatorial vibrations)

4	892	914	Localized on uranyl 1 (2 x I coordination)
4	905		Localized on uranyl 2 (Ag in 2nd coordination sphere)

Table S6 Natural Energy Decomposition Analysis for monomeric version of **1**, $[UO_2Ag(C_7H_4IO_2)_2(NO_3)]$.

Ligand	Bond Length (Å)	Electrical (kcal/mol)	Charge Transfer (kcal/mol)	Core (kcal/mol)	Total Energy (kcal/mol)
Ag^+	n/a	-185.25	-94.51	134.11	-145.66
o-IBA, aver.	2.726984	-66.47	-141.79	227.08	18.82
O^{2-}	1.733555	-337.19	-746.89	939.15	-144.94

Table S7 Wiberg bond index for selected bonds in **1**.

Group	Bond	Bond Index
UO_2	U1-O1	2.0791
UO_2	U1-O2	1.9961
U-benzoate	U1-O3	0.3839
U-benzoate	U1-O4	0.4075
U-benzoate	U1-O7	0.4051
U-benzoate	U1-O8	0.3782
U-nitrate	U1-O5	0.3834
U-nitrate	U1-O6	0.3793
Ag	Ag1-O2	0.0517
Ag	Ag1-I1	0.2224
Ag	Ag1-I2	0.2383
Ag	Ag1-O3	0.0316
Ag	Ag1-O8	0.0402

Table S8 Wiberg bond index for selected bonds in **2**.

Group	Bond	Bond Index
UO_2	U1-O1	2.0470
UO_2	U1-O2	2.0499
U-benzoate	U1-O3	0.4202
U-benzoate	U1-O4	0.3424
U-benzoate	U1-O5	0.3599
U-benzoate	U1-O6	0.3876
U-benzoate	U1-O7	0.4007
U-benzoate	U1-O8	0.4067
Ag	Ag1-I1	0.2272
Ag	Ag1-I3	0.1546
Ag	Ag1-O4	0.0554
Ag	Ag1-O5	0.0580

Table S9 Wiberg bond index for selected bonds in **3**.

Subunit	Group	Bond	Bond Index
$U(benzoate)_2$-Ag	UO_2	U1-O1	2.0465
	UO_2	U1-O2	2.0447
	U-benzoate	U1-O3	0.4328
	U-benzoate	U1-O4	0.4141
	U-benzoate	U1-O5	0.4006
	U-benzoate	U1-O6	0.3728
	U-benzoate	U1-O7	0.3928
	U-benzoate	U1-O8	0.3963
	Ag	Ag1-O2	0.0766
	Ag	Ag1-O6	0.0502
	Ag	Ag1-O7	0.0443
	Ag	Ag1-I1	0.2428
$U(benzoate)_3^-$	UO_2	U1-O1	2.0645
	UO_2	U1-O2	1.9087
	U-benzoate	U1-O3	0.4133
	U-benzoate	U1-O4	0.4105
	U-benzoate	U1-O5	0.4080
	U-benzoate	U1-O6	0.4354
	U-benzoate	U1-O7	0.4330
	U-benzoate	U1-O8	0.4156

Table S10 Wiberg bond index for selected bonds in **4**.

Subunit	Group	Bond	Bond Index
$U(benzoate)_2$-Ag	UO_2	U1-O1	2.067
	UO_2	U1-O2	2.057
	U-benzoate	U1-O5	0.4133
	U-benzoate	U1-O6	0.3934
	U-benzoate	U1-O7	0.3825
	U-benzoate	U1-O8	0.3967
	U-benzoate	U1-O9	0.3417
	U-benzoate	U1-O10	0.3816
AgO_2I_3 center	Ag	Ag1-O8	0.0306
	Ag	Ag1-O9	0.0515
	Ag	Ag1-I1	0.2182
	Ag	Ag1-I3	0.1620
	Ag	Ag1-I5	0.1604
UO_2-Ag	UO_2	U1-O1	2.0671
	UO_2	U1-O2	1.9824
	U-benzoate	U1-O5	0.3909
	U-benzoate	U1-O6	0.3871
	U-benzoate	U1-O7	0.4291
	U-benzoate	U1-O8	0.4131
	U-benzoate	U1-O9	0.3794
	U-benzoate	U1-O10	0.3839

Table S11 Topological parameters of **1**. ρ_{BCP} = magnitude of electron density at the bond critical point; $\nabla^2\rho$ = Laplacian of electron density at the bond critical point; ε = deviation from cylindrical symmetry of electron cloud; $G(\mathbf{r}_b)$ = kinetic energy density of bond or non-covalent interaction; $V(\mathbf{r}_b)$ = potential energy density of bond or non-covalent interaction; δ_{AB} = delocalization index of bond or non-covalent interaction.

Atoms	ρ_{BCP}	$\nabla^2\rho$	ε	$G(\mathbf{r}_b)$	$V(\mathbf{r}_b)$	-V/G	δ_{AB}
U1-O1	0.3250	0.2944	0.0021	0.3834	-0.6932	1.8081	1.9056
U1-O2	0.3242	0.3302	0.0054	0.3915	-0.7006	1.7893	1.8346
U1-O3	0.0613	0.1907	0.1451	0.0564	-0.0651	1.1548	0.3377
U1-O4	0.0630	0.1936	0.1420	0.0578	-0.0672	1.1627	0.3534
U1-O5	0.0572	0.1813	0.1896	0.0525	-0.0596	1.1362	0.3064
U1-O6	0.0565	0.1807	0.1883	0.0520	-0.0588	1.1311	0.2992
U1-O7	0.0644	0.1969	0.1460	0.0591	-0.0690	1.1672	0.3591
U1-O8	0.0602	0.1883	0.1474	0.0554	-0.0637	1.1500	0.3324
Ag1-O2	0.0340	0.1497	0.0220	0.0381	-0.0389	1.0188	0.2143
Ag1-O3	0.0319	0.1396	0.0509	0.0358	-0.0366	1.0243	0.1837
Ag1-O8	0.0395	0.1800	0.0291	0.0469	-0.0488	1.0404	0.2248
Ag1-I1	0.0520	0.1283	0.0332	0.0403	-0.0510	1.2661	0.5593
Ag1-I2	0.0557	0.1361	0.0179	0.0435	-0.0558	1.2838	0.5941

Table S12 Topological parameters of **2**. ρ_{BCP} = magnitude of electron density at the bond critical point; $\nabla^2\rho$ = Laplacian of electron density at the bond critical point; ε = deviation from cylindrical symmetry of electron cloud; $G(\mathbf{r}_b)$ = kinetic energy density of bond or non-covalent interaction; $V(\mathbf{r}_b)$ = potential energy density of bond or non-covalent interaction; δ_{AB} = delocalization index of bond or non-covalent interaction.

Atoms	ρ_{BCP}	$\nabla^2\rho$	ε	$G(\mathbf{r}_b)$	$V(\mathbf{r}_b)$	-V/G	δ_{AB}
U1-O1	0.3090	0.3156	0.0028	0.3588	-0.6388	1.7802	1.8689
U1-O2	0.3249	0.3007	0.0022	0.3846	-0.6941	1.8046	1.8961
U1-O3	0.0633	0.1902	0.1494	0.0572	-0.0669	1.1691	0.3646
U1-O4	0.0521	0.1720	0.1109	0.0484	-0.0538	1.1115	0.2834
U1-O5	0.0551	0.1762	0.1341	0.0505	-0.0570	1.1278	0.3077
U1-O6	0.0583	0.1813	0.1408	0.0530	-0.0607	1.1451	0.3280
U1-O7	0.0612	0.1885	0.1416	0.0559	-0.0647	1.1571	0.3482
U1-O8	0.0611	0.1887	0.1402	0.0559	-0.0646	1.1556	0.3379
Ag1-I1	0.0449	0.0999	0.0368	0.0312	-0.0392	1.2562	0.5237
Ag1-I3	0.0331	0.0763	0.0773	0.0219	-0.0257	1.1766	0.3809
Ag1-O4	0.0380	0.1689	0.0254	0.0438	-0.0453	1.0352	0.2370
Ag1-O5	0.0454	0.2104	0.0197	0.0551	-0.0577	1.0459	0.2830
I3-O2	0.0081	0.0284	0.0921	0.0056	-0.0042	0.7507	0.0711
O1-H5	0.0066	0.0259	0.3004	0.0051	-0.0037	0.731	0.0222
O1-H20	0.0063	0.0239	0.0796	0.0047	-0.0035	0.7331	0.0268
O2-H12	0.0073	0.0301	1.0094	0.006	-0.0044	0.7341	0.0192
O2-H13	0.0065	0.0249	0.0781	0.0049	-0.0036	0.7263	0.029

Table S13 Topological parameters of **3**. ρ_{BCP} = magnitude of electron density at the bond critical point; $\nabla^2\rho$ = Laplacian of electron density at the bond critical point; ε = deviation from cylindrical symmetry of electron cloud; $G(\mathbf{r}_b)$ = kinetic energy density of bond or non-covalent interaction; $V(\mathbf{r}_b)$ = potential energy density of bond or non-covalent interaction; δ_{AB} = delocalization index of bond or non-covalent interaction.

Atoms	ρ_{BCP}	$\nabla^2\rho$	ε	$G(\mathbf{r}_b)$	$V(\mathbf{r}_b)$	-V/G	δ_{AB}
U1-O1	0.3055	0.3181	0.0009	0.3526	-0.6257	1.7745	1.8682
U1-O2	0.2910	0.3252	0.0038	0.3287	-0.5760	1.7526	1.8590
U1-O3	0.0659	0.1996	0.1545	0.0605	-0.0711	1.1748	0.3746
U1-O4	0.0631	0.1940	0.1476	0.0580	-0.0674	1.1632	0.3587
U1-O5	0.0600	0.1873	0.1366	0.0551	-0.0633	1.1496	0.3325
U1-O6	0.0569	0.1819	0.1340	0.0525	-0.0595	1.1333	0.3100
U1-O7	0.0617	0.1933	0.1399	0.0570	-0.0657	1.1520	0.3367
U1-O8	0.0595	0.1843	0.1360	0.0542	-0.0623	1.1500	0.3334
Ag1-O2	0.0448	0.2013	0.0147	0.0529	-0.0554	1.0482	0.2906
Ag1-O6	0.0420	0.1912	0.0279	0.0500	-0.0521	1.0434	0.2614
Ag1-O7	0.0398	0.1817	0.0164	0.0472	-0.0489	1.0370	0.2426
Ag1-I1	0.0551	0.1214	0.0641	0.0399	-0.0523	1.3105	0.6212
U1-O1	0.3061	0.3049	0.0008	0.3499	-0.6235	1.7822	1.8890
U1-O2	0.2848	0.3652	0.0050	0.3296	-0.5678	1.7230	1.7336
U1-O3	0.0583	0.1750	0.1329	0.0516	-0.0594	1.1521	0.3421
U1-O4	0.0604	0.1847	0.1390	0.0547	-0.0631	1.1553	0.3454
U1-O5	0.0597	0.1831	0.1330	0.0540	-0.0622	1.1520	0.3401
U1-O6	0.0628	0.1874	0.1384	0.0563	-0.0657	1.1671	0.3618
U1-O7	0.0660	0.1991	0.1559	0.0604	-0.0710	1.758	0.3763
U1-O8	0.0632	0.1936	0.1505	0.0579	-0.0674	1.1639	0.3598
O1-H20	0.0048	0.0181	0.0967	0.0035	-0.0025	0.7099	0.0216
O2-H14	0.0044	0.0166	0.0495	0.0032	-0.0023	0.7071	0.0193

Table S14 Topological parameters of **4**. ρ_{BCP} = magnitude of electron density at the bond critical point; $\nabla^2\rho$ = Laplacian of electron density at the bond critical point; ε = deviation from cylindrical symmetry of electron cloud; $G(\mathbf{r}_b)$ = kinetic energy density of bond or non-covalent interaction; $V(\mathbf{r}_b)$ = potential energy density of bond or non-covalent interaction; δ_{AB} = delocalization index of bond or non-covalent interaction.

Atoms	ρ_{BCP}	$\nabla^2\rho$	ε	$G(\mathbf{r}_b)$	$V(\mathbf{r}_b)$	-V/G	δ_{AB}
U1-O1	0.3225	0.3002	0.0013	0.3800	-0.6849	1.8026	1.8970
U1-O2	0.3025	0.3193	0.0001	0.3479	-0.6160	1.7706	1.8686
U1-O5	0.0634	0.1942	0.1477	0.0581	-0.0677	1.1646	0.3577
U1-O6	0.0596	0.1829	0.1385	0.0541	-0.0624	1.1538	0.3397
U1-O7	0.0613	0.1901	0.1455	0.0562	-0.0650	1.1551	0.3417
U1-O8	0.0609	0.1896	0.1325	0.0560	-0.0645	1.1526	0.3372
U1-O9	0.0534	0.1707	0.1233	0.0486	-0.0546	1.1223	0.2962
U1-O10	0.0580	0.1808	0.1255	0.0528	-0.0605	1.1444	0.3256
Ag1-O8	0.0257	0.1109	0.0235	0.0278	-0.0278	1.0014	0.1510
Ag1-O9	0.0418	0.1950	0.0155	0.0508	-0.0528	1.0397	0.2526
Ag1-I1	0.0454	0.1089	0.0699	0.0335	-0.0415	1.2403	0.5412
Ag1-I3	0.0386	0.0991	0.0886	0.0289	-0.0343	1.1895	0.4231
Ag1-I5	0.0404	0.1047	0.0936	0.0307	-0.0367	1.1967	0.4213
U1-O1	0.3242	0.2971	0.0016	0.3821	-0.6900	1.8057	1.8992
U1-O2	0.3011	0.3227	0.0062	0.3467	-0.6127	1.7674	1.8100
U1-O5	0.0581	0.1798	0.1388	0.0526	-0.0602	1.1452	0.3327
U1-O6	0.0589	0.1825	0.1353	0.0536	-0.0616	1.1488	0.3330
U1-O7	0.0662	0.2003	0.1582	0.0607	-0.0713	1.1752	0.3727
U1-O8	0.0618	0.1859	0.1346	0.0556	-0.0647	1.1639	0.3540
U1-O9	0.0574	0.1802	0.1237	0.0524	-0.0598	1.1406	0.3227
U1-O10	0.0543	0.1649	0.1260	0.0478	-0.0543	1.1372	0.3203
I3-O2	0.0072	0.0277	0.2968	0.0053	-0.0038	0.7253	0.0611
I5-O2	0.0135	0.0534	0.0853	0.0109	-0.0091	0.8339	0.1084

II. Powder X-ray diffraction data

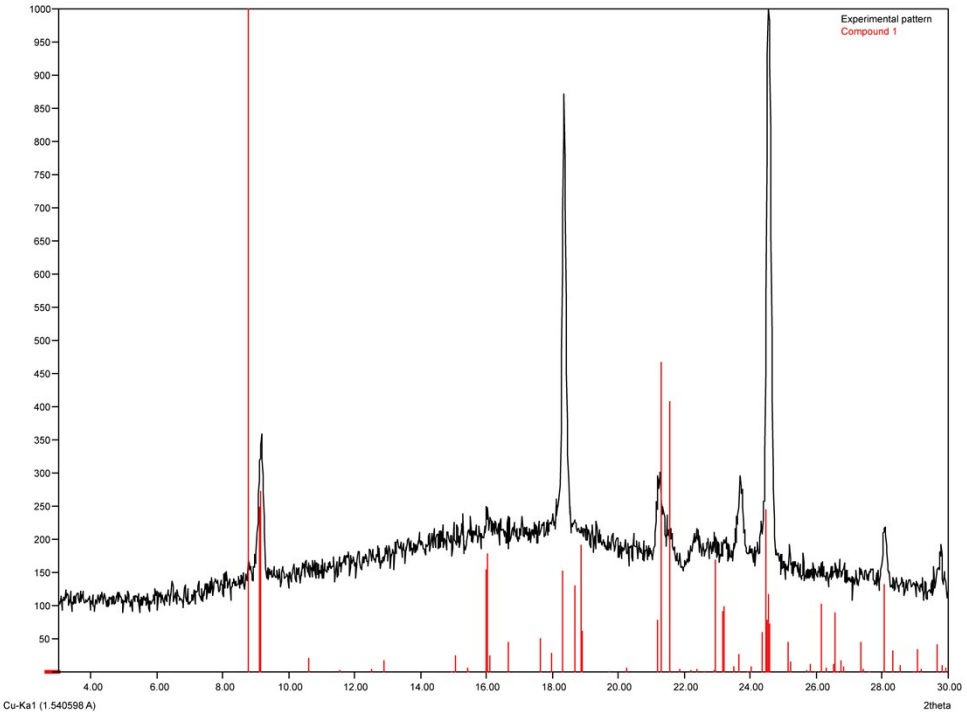

Figure S5 The observed PXRD pattern of **1** with calculated pattern overlaid in red.

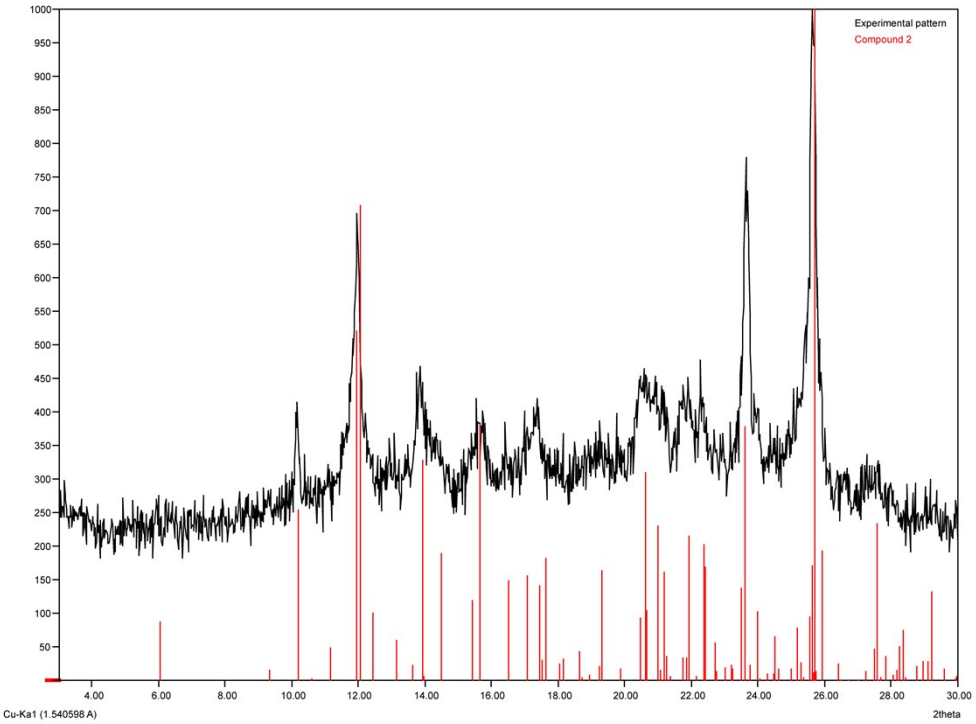

Figure S6 The observed PXRD pattern of **2** with calculated pattern overlaid in red.

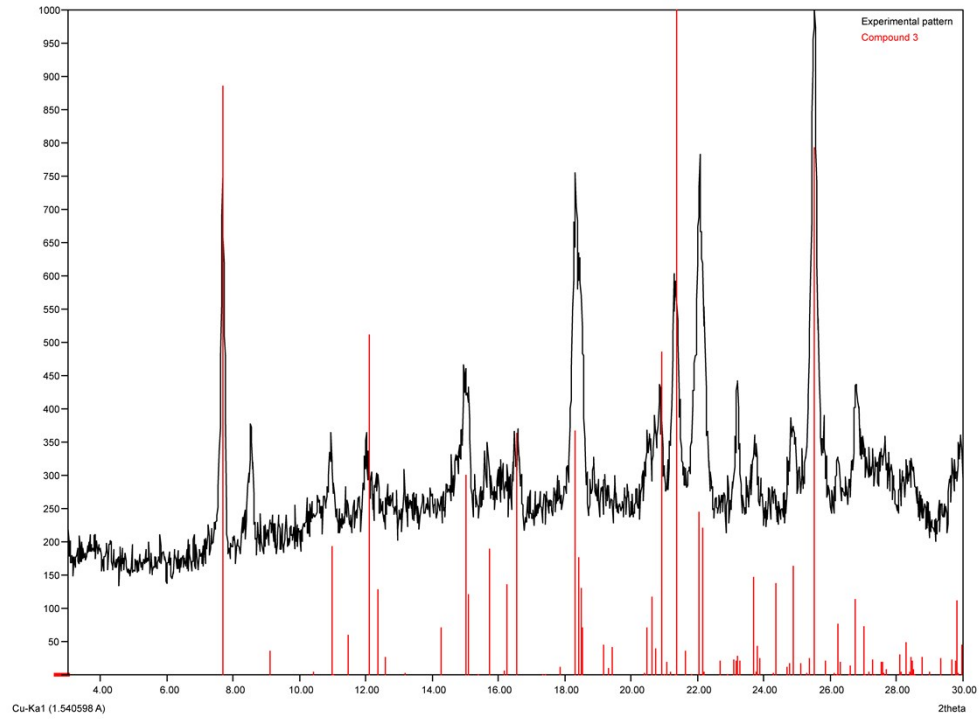

Figure S7 The observed PXRD pattern of **3** with calculated pattern overlaid in red. We acknowledge one unidentified impurity at ca. 8.5 degrees 2-theta.

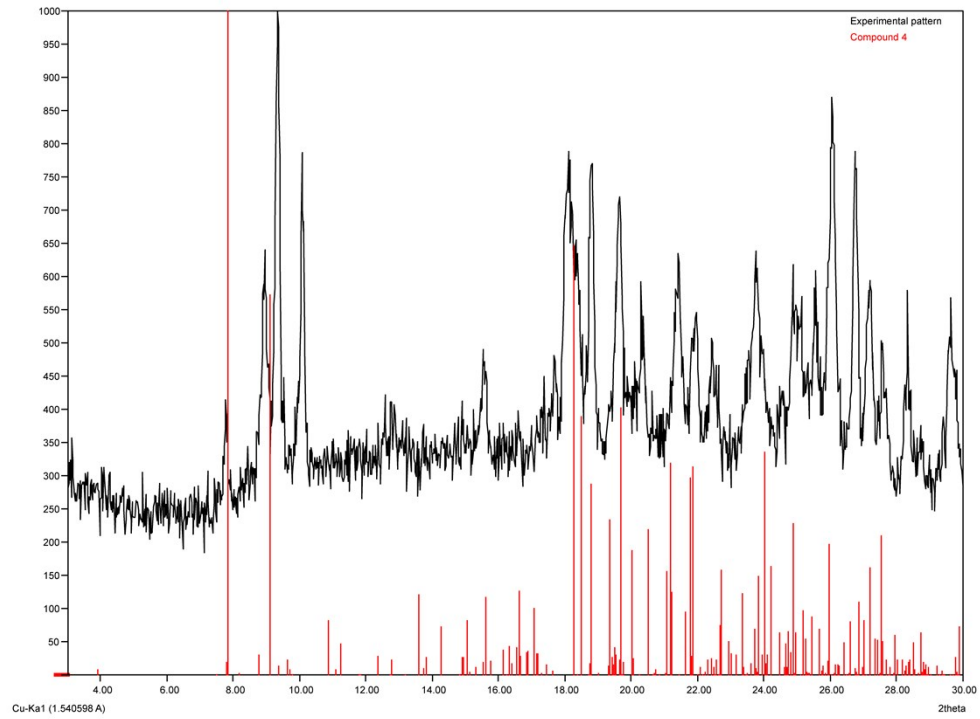

Figure S8 The observed PXRD pattern of **4** with calculated pattern overlaid in red. We acknowledge one unidentified impurity at ca. 10 degrees 2-theta.

III. Thermal Ellipsoid Plots

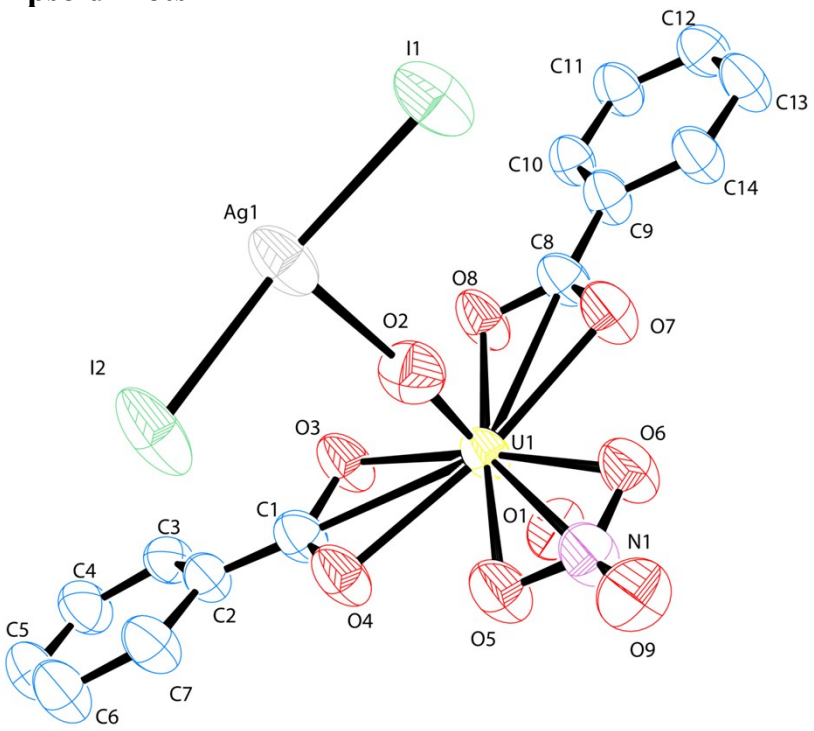

Figure S9 ORTEP illustration of **1**. Ellipsoids are shown at 50% probability level.

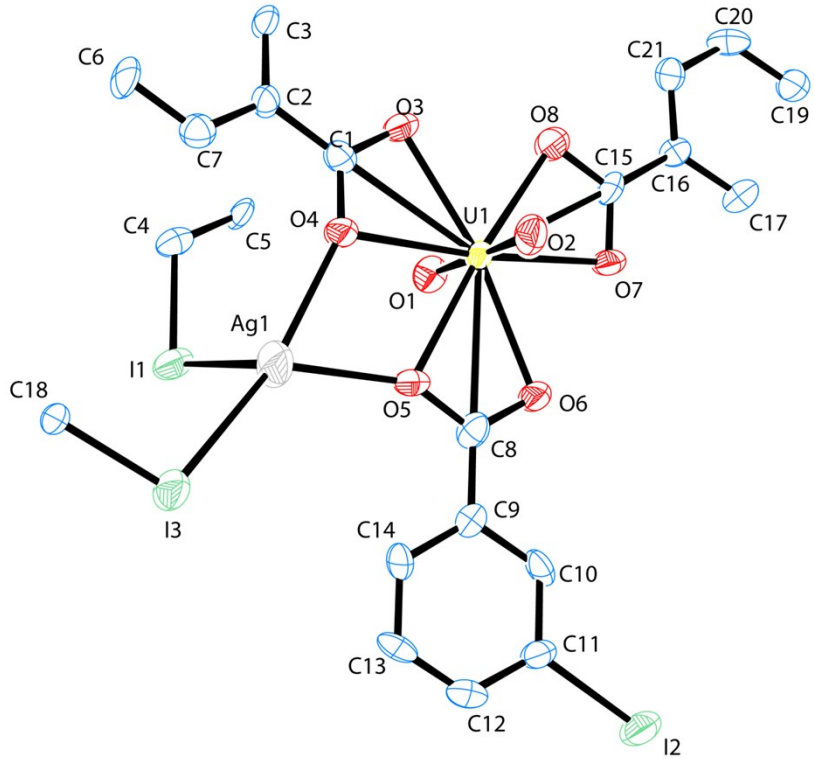

Figure S10 ORTEP illustration of **2**. Ellipsoids are shown at 50% probability level.

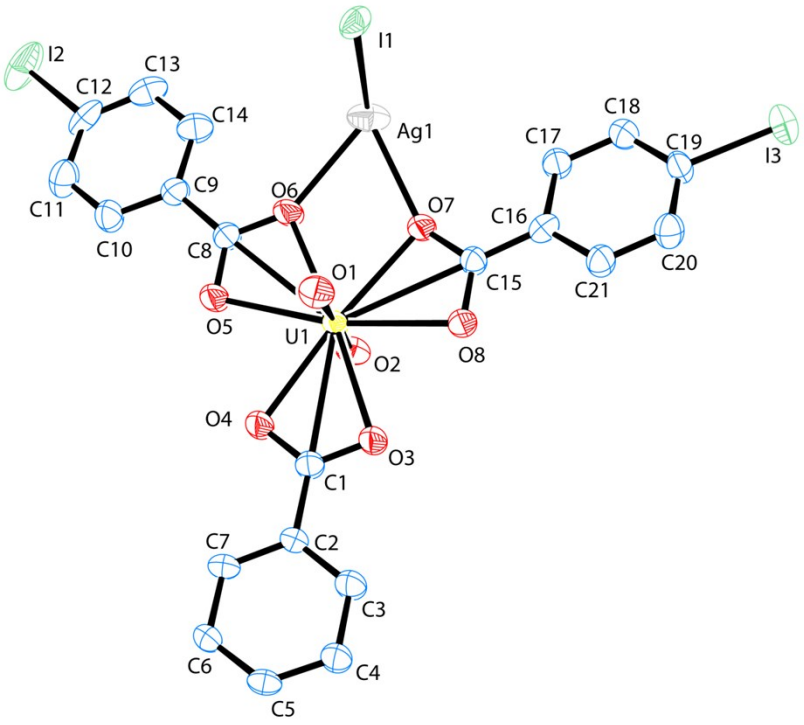

Figure S11 ORTEP illustration of **3**. Ellipsoids are shown at 50% probability level.

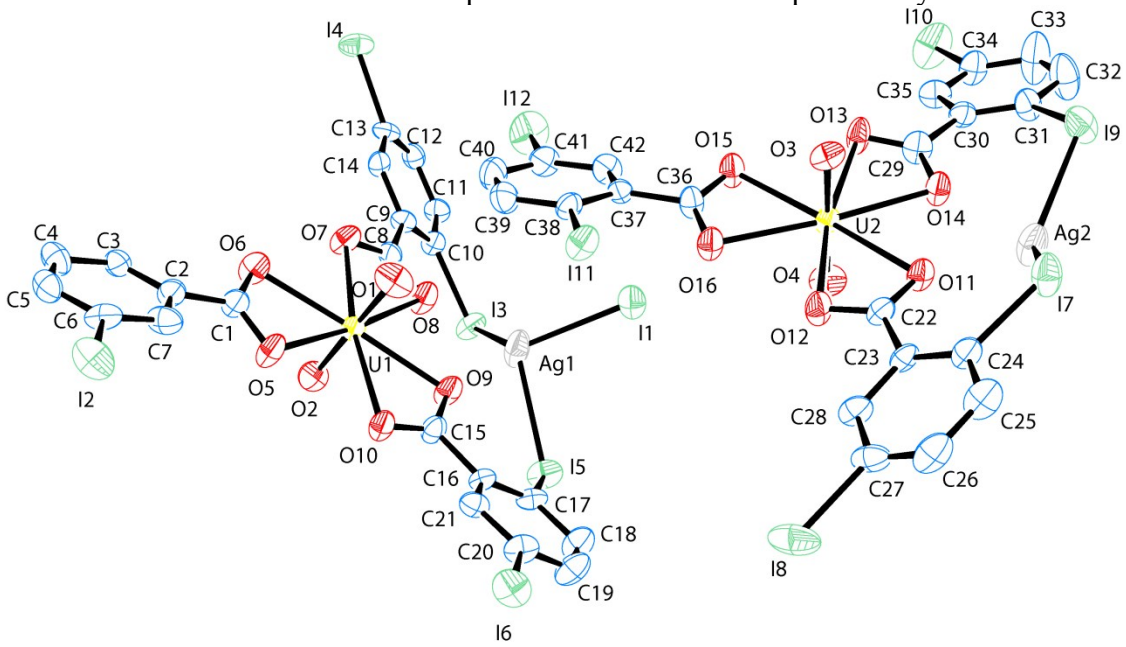

Figure S12 ORTEP illustration of **4**. Ellipsoids are shown at 50% probability level.

IV. Tables of Bond Distances

Table S15 U-O equatorial bond lengths in **1-4**.

Compound	d_{U1-O3} [Å]	d_{U1-O4} [Å]	d_{U1-O5} [Å]	d_{U1-O6} [Å]	d_{U1-O7} [Å]	d_{U1-O8} [Å]	d_{U1-O9} [Å]	d_{U1-O10} [Å]
1	2.458 (6)	2.433 (6)	2.485 (6)	2.482 (6)	2.443 (6)	2.451 (6)		
2	2.454 (6)	2.514 (6)	2.494 (6)	2.474 (6)	2.455 (6)	2.444 (6)		
3	2.441 (4)	2.423 (4)	2.466 (4)	2.446 (4)	2.479 (4)	2.460 (4)		
4			2.422 (5)	2.471 (5)	2.475 (5)	2.511 (5)	2.454 (5)	2.481 (5)

Table S16 Additional U-O equatorial bond lengths in **4**.

Compound	d_{U2-O11} [Å]	d_{U2-O12} [Å]	d_{U2-O13} [Å]	d_{U2-O14} [Å]	d_{U2-O15} [Å]	d_{U2-O16} [Å]
4	2.509 (5)	2.451 (5)	2.477 (5)	2.454 (5)	2.439 (5)	2.467 (5)

Table S17 Ag-O bond lengths in **1-4**.

Compound	d_{Ag1-O2} [Å]	d_{Ag1-O3} [Å]	d_{Ag1-O4} [Å]	d_{Ag1-O5} [Å]	d_{Ag1-O6} [Å]	d_{Ag1-O7} [Å]	d_{Ag1-O8} [Å]	d_{Ag1-O9} [Å]	$d_{Ag2-O11}$ [Å]	$d_{Ag2-O14}$ [Å]
1	2.464 (7)	2.403 (6)					2.500 (6)			
2			2.413 (6)	2.339 (6)						
3	2.343 (4)				2.397 (4)	2.375 (4)				
4							2.368 (5)	2.632 (6)	2.375 (5)	2.594 (5)

Table S18 Ag-I Bond Lengths in **1-4**.

Com-pound	d_{Ag1-I1} [Å]	d_{Ag1-I2} [Å]	d_{Ag1-I3} [Å]	d_{Ag1-I5} [Å]	d_{Ag2-I7} [Å]	d_{Ag2-I9} [Å]	$d_{Ag2-I11}$ [Å]
1	2.7213 (10)	2.6848 (10)					
2	2.9750 (15)		2.820 (2)				
3	2.7000 (7)						
4	2.7799 (14)		2.8754 (15)	2.8734 (10)	2.8815 (12)	2.8540 (9)	2.8097 (17)

V. DFT Computed Structure Coordinates

Table S19 Crystallographically-derived Cartesian coordinates for model structure of **1**. All units are in Angstroms.

U	9.623979	-3.302818	16.883611
I	11.817359	-3.568341	11.71316
Ag	5.636002	-2.861406	15.63745
I	11.460284	1.014143	13.799418
O	7.958295	-3.048455	16.439999
O	11.292593	-3.548604	17.337095
O	10.223654	-1.215482	15.74516
O	10.273491	-3.59107	14.529676
O	9.667102	-1.050614	17.82774
O	9.569531	-5.350872	15.571934
O	8.930819	-3.408355	19.263869
O	8.904519	-5.27866	18.208063
C	10.07581	-5.654612	13.290967
C	10.082319	-0.50152	16.778708
C	10.913558	1.705265	15.730644
C	10.759331	-5.352736	12.109354
C	9.975973	-4.833315	14.496773
C	10.39065	0.950114	16.774837
C	11.162536	3.0493	15.874837
H	11.497407	3.534335	15.155805
C	9.427544	-6.890717	13.33258
H	8.952284	-7.120277	14.098063
C	10.416888	2.966918	18.111289
H	10.260188	3.3897	18.92516
C	10.823148	-6.276895	11.068064
H	11.307132	-6.074412	10.299677
C	10.142373	1.648367	17.972902
H	9.777472	1.18803	18.692902
C	10.18117	-7.474985	11.165806
H	10.23132	-8.085408	10.466128
O	8.176927	-5.179031	20.267418
C	9.467062	-7.78143	12.28258
H	9.006863	-8.58805	12.337741
N	8.647755	-4.656969	19.294837
C	10.923127	3.679999	17.062257
H	11.102525	4.5872	17.156128
U	6.997341	-1.155799	12.148644
I	4.803961	-0.890276	17.319095

Ag	10.985318	-1.59721	13.394805
I	5.161036	-5.47276	15.232837
O	8.663025	-1.410161	12.592257
O	5.328727	-0.910012	11.69516
O	6.397666	-3.243135	13.287096
O	6.347829	-0.867546	14.502579
O	6.954218	-3.408003	11.204515
O	7.051788	0.892256	13.460321
O	7.6905	-1.050262	9.768386
O	7.716801	0.820044	10.824193
C	6.54551	1.195995	15.741289
C	6.539	-3.957096	12.253547
C	5.707762	-6.163881	13.301612
C	5.861989	0.894119	16.922902
C	6.645346	0.374699	14.535483
C	6.23067	-5.408731	12.257418
C	5.458783	-7.507916	13.157418
H	5.123913	-7.992951	13.87645
C	7.193776	2.432101	15.699676
H	7.669036	2.66166	14.934192
C	6.204432	-7.425535	10.920967
H	6.361132	-7.848316	10.107096
C	5.798172	1.818279	17.964192
H	5.314188	1.615796	18.732579
C	6.478947	-6.106983	11.059354
H	6.843847	-5.646646	10.339354
C	6.44015	3.016369	17.86645
H	6.39	3.626791	18.566127
O	8.444392	0.720415	8.764838
C	7.154258	3.322813	16.749676
H	7.614457	4.129433	16.694515
N	7.973565	0.198352	9.737419
C	5.698193	-8.138616	11.969999
H	5.518795	-9.045816	11.876128

Table S20 Crystallographically-derived Cartesian coordinates for model structure of **2**. All units are in Angstroms.

U	2.112768	2.492553	10.970928
I	-2.798809	8.738135	12.285506
I	-0.29451	-3.363185	6.076995
I	6.553405	6.954114	16.070776

Ag	5.455416	0.167265	11.235278
O	0.858815	4.559711	11.395646
O	1.36192	1.748653	12.387145
O	1.242415	0.703409	9.534206
O	-0.116579	3.049104	10.139064
O	3.368726	3.985409	12.492593
O	3.179256	0.277814	10.442226
O	4.392646	2.135417	11.917025
O	2.846273	3.215615	9.560568
C	7.738809	4.452204	14.875412
H	8.476379	4.72413	15.371894
C	6.586046	5.202483	14.900309
C	-3.500493	5.443216	9.57082
H	-4.156511	5.215816	8.952781
C	3.324965	-3.492509	8.46948
H	4.016694	-4.097286	8.611541
C	1.255482	-1.676288	8.065265
H	0.571149	-1.065339	7.910023
C	3.2926	-2.274956	9.169534
H	3.969632	-2.066824	9.771463
C	-1.465337	6.210691	11.312167
H	-0.778495	6.490472	11.873089
C	5.55439	3.657719	13.37425
C	-1.348329	5.020274	10.594539
C	5.491829	4.819822	14.127028
H	4.722684	5.341731	14.116776
C	7.808066	3.312399	14.127028
H	8.583072	2.797106	14.127028
C	4.402241	3.258448	12.564356
C	2.319439	-3.781024	7.565854
H	2.340514	-4.570239	7.07523
C	1.286114	-2.888064	7.403289
C	2.26503	-1.394688	8.964497
C	-2.616911	6.974207	11.180358
C	-2.368075	4.621179	9.750959
H	-2.307855	3.810565	9.299878
C	-0.14914	4.166027	10.755639
C	-3.620898	6.589864	10.329456
H	-4.390265	7.108394	10.262086
C	6.733951	2.937583	13.380109
H	6.795913	2.171618	12.855801
C	2.235743	-0.066868	9.687984
I	7.855966	-0.875534	12.285506

I	6.623759	0.778387	8.568483
I	-0.821034	-0.875534	12.285506
O	11.513589	-5.053958	11.395646
O	10.538195	-6.564565	10.139064
C	7.154281	-4.170453	9.57082
H	6.498264	-4.397853	8.952781
C	9.189438	-3.402978	11.312167
H	9.876279	-3.123197	11.873089
C	9.306446	-4.593395	10.594539
C	8.037864	-2.639462	11.180358
C	8.2867	-4.99249	9.750959
H	8.34692	-5.803104	9.299878
C	10.505635	-5.447642	10.755639
C	7.033877	-3.023805	10.329456
H	6.264509	-2.505275	10.262086
I	4.12732	-2.510041	13.22018
O	7.311998	0.458664	16.798363
O	6.288079	2.308656	17.37393
C	2.941916	-0.008131	14.415544
H	2.204346	-0.280057	13.919062
C	4.094679	-0.75841	14.390647
C	5.126335	0.786354	15.916705
C	5.188896	-0.375749	15.163928
H	5.95804	-0.897658	15.17418
C	2.872658	1.131674	15.163928
H	2.097653	1.646967	15.163928
C	6.278484	1.185625	16.7266
C	3.946773	1.50649	15.910847
H	3.884812	2.272455	16.435155
U	4.090543	-7.121116	10.970928
I	1.683265	-12.976854	6.076995
I	8.53118	-2.659555	16.070776
O	2.836589	-5.053958	11.395646
O	3.339695	-7.865016	12.387145
O	3.22019	-8.91026	9.534206
O	1.861195	-6.564565	10.139064
O	5.346501	-5.62826	12.492593
O	5.157031	-9.335855	10.442226
O	6.370421	-7.478252	11.917025
O	4.824048	-6.398054	9.560568
C	9.716583	-5.161465	14.875412
H	10.454154	-4.889539	15.371894
C	8.563821	-4.411186	14.900309

C	-1.522719	-4.170453	9.57082
H	-2.178736	-4.397853	8.952781
C	5.302739	-13.106178	8.46948
H	5.994468	-13.710955	8.611541
C	3.233257	-11.289957	8.065265
H	2.548924	-10.679008	7.910023
C	5.270374	-11.888625	9.169534
H	5.947407	-11.680493	9.771463
C	0.512438	-3.402978	11.312167
H	1.199279	-3.123197	11.873089
C	7.532164	-5.95595	13.37425
C	0.629446	-4.593395	10.594539
C	7.469604	-4.793847	14.127028
H	6.700459	-4.271938	14.116776
C	9.785841	-6.30127	14.127028
H	10.560847	-6.816563	14.127028
C	6.380015	-6.355221	12.564356
C	4.297214	-13.394693	7.565854
H	4.318289	-14.183908	7.07523
C	3.263888	-12.501733	7.403289
C	4.242805	-11.008357	8.964497
C	-0.639136	-2.639462	11.180358
C	-0.3903	-4.99249	9.750959
H	-0.33008	-5.803104	9.299878
C	1.828635	-5.447642	10.755639
C	-1.643123	-3.023805	10.329456
H	-2.412491	-2.505275	10.262086
C	8.711726	-6.676086	13.380109
H	8.773687	-7.442051	12.855801
C	4.213517	-9.680537	9.687984
O	5.086835	-3.288207	5.111272
O	3.149994	-2.862612	4.203252
C	3.004285	0.907711	6.175998
H	2.312556	1.512488	6.033937
C	5.073767	-0.90851	6.580213
H	5.7581	-1.519459	6.735455
C	3.03665	-0.309842	5.475944
H	2.359618	-0.517974	4.874015
C	4.009811	1.196226	7.079624
H	3.988736	1.985441	7.570248
C	5.043136	0.303266	7.242189
C	4.06422	-1.19011	5.680981
C	4.093507	-2.51793	4.957494

Table S21 Crystallographically-derived Cartesian coordinates for model structure of **3**. All units are in Angstroms.

U	4.793659	0.980467	16.999788
I	11.922144	5.51843	13.468784
I	4.618352	-8.230116	16.994362
Ag	1.389135	-1.083674	17.743392
I	-2.552632	5.115323	20.554048
O	3.745259	-1.21647	17.47285
O	4.155769	0.942014	15.346883
O	5.722773	-1.257925	16.57944
O	3.440274	2.978995	17.50192
O	2.472824	1.054941	17.769361
O	5.396739	1.012058	18.688159
O	6.020332	2.999007	16.457347
O	7.098285	1.116408	16.207347
C	9.351806	2.4358	15.104635
H	9.394151	1.510939	15.19572
C	4.719837	-1.892605	16.99223
C	7.06301	2.370045	16.093006
C	1.121687	4.36843	18.403081
H	1.811129	4.881606	18.050369
C	10.330244	4.478498	14.405024
C	4.60438	-6.139531	16.926339
C	8.176273	4.494222	15.41665
H	7.429959	4.960226	15.717038
C	8.215863	3.120511	15.534867
C	0.030555	4.993104	18.982538
H	-0.025427	5.920823	19.011608
C	-0.944014	2.846055	19.436026
H	-1.652935	2.342885	19.765483
C	1.195987	2.984712	18.34688
C	9.235229	5.190369	14.852698
H	9.20818	6.116659	14.779054
C	5.646751	-4.095403	16.282929
H	6.33295	-3.647982	15.843007
C	3.610002	-5.440525	17.577501
H	2.927859	-5.899381	18.011609
C	-0.974249	4.20976	19.517421
C	0.154573	2.212804	18.854631
H	0.190682	1.285085	18.80812
C	2.418003	2.327161	17.848818
C	4.66741	-3.356372	16.941843

C	5.620338	-5.464826	16.267425
H	6.281561	-5.939406	15.817813
C	3.628964	-4.063955	17.581377
H	2.94983	-3.596521	18.011609
C	10.419916	3.120511	14.540682
H	11.18048	2.664513	14.259675
I	-0.160956	-1.62887	15.600953
O	1.130345	-1.012058	20.071491
U	1.733424	-0.980467	21.759861
I	-5.395061	-5.51843	25.290865
I	1.908731	8.230116	21.765287
I	9.079715	-5.115323	18.205601
O	2.781825	1.21647	21.286799
O	2.371315	-0.942014	23.412766
O	0.80431	1.257925	22.180209
O	3.086809	-2.978995	21.25773
O	4.05426	-1.054941	20.990288
O	0.506752	-2.999007	22.302302
O	-0.571202	-1.116408	22.552302
C	-2.824723	-2.4358	23.655014
H	-2.867067	-1.510939	23.563929
C	1.807247	1.892605	21.767419
C	-0.535926	-2.370045	22.666643
C	5.405396	-4.36843	20.356568
H	4.715955	-4.881606	20.709281
C	-3.80316	-4.478498	24.354626
C	1.922704	6.139531	21.83331
C	-1.649189	-4.494222	23.342999
H	-0.902875	-4.960226	23.042611
C	-1.688779	-3.120511	23.224782
C	6.496528	-4.993104	19.777111
H	6.55251	-5.920823	19.748041
C	7.471098	-2.846055	19.323623
H	8.180019	-2.342885	18.994166
C	5.331097	-2.984712	20.412769
C	-2.708145	-5.190369	23.906952
H	-2.681096	-6.116659	23.980595
C	0.880333	4.095403	22.476721
H	0.194134	3.647982	22.916643
C	2.917082	5.440525	21.182148
H	3.599225	5.899381	20.74804
C	7.501333	-4.20976	19.242228
C	6.372511	-2.212804	19.905018

H	6.336402	-1.285085	19.951529
C	4.109081	-2.327161	20.910831
C	1.859673	3.356372	21.817807
C	0.906745	5.464826	22.492224
H	0.245522	5.939406	22.941836
C	2.89812	4.063955	21.178272
H	3.577254	3.596521	20.74804
C	-3.892833	-3.120511	24.218967
H	-4.653396	-2.664513	24.499974
O	5.740856	-4.148293	12.61239
O	4.662903	-6.030892	12.86239
C	2.409382	-4.7115	13.965102
H	2.367037	-5.636361	13.874016
C	4.698178	-4.777255	12.976731
C	1.430944	-2.668802	14.664713
C	3.584915	-2.653078	13.653086
H	4.331229	-2.187074	13.352699
C	3.545325	-4.026789	13.534869
C	2.525959	-1.956931	14.217039
H	2.553008	-1.030641	14.290683
C	1.341271	-4.026789	14.529054
H	0.580708	-4.482787	14.810062

Table S22 Crystallographically-derived Cartesian coordinates for model structure of **4**. All units are in Angstroms.

U	14.657954	15.199538	17.089507
I	11.506884	18.616768	14.127904
I	15.110895	15.303711	9.162606
I	19.7927	15.010395	15.394626
I	11.351438	13.341941	23.955786
I	9.886701	17.486724	18.563903
I	20.024521	11.422412	21.355815
O	14.959331	15.403174	14.640571
O	16.94032	14.523382	16.42513
O	16.423704	14.389822	18.535583
O	12.427246	15.775185	17.933239
O	15.225514	16.865029	17.333142
O	13.889985	15.180701	19.448091
O	14.085943	13.563694	16.86565
O	13.043895	16.080809	15.380017
C	19.77699	13.974187	17.234249
C	9.735373	15.223506	22.201345

H	9.103797	15.134308	22.877859
C	19.929205	12.542182	19.591934
C	17.271085	14.235252	17.598353
C	18.618246	13.717336	17.948972
C	10.944071	14.579758	22.300238
C	14.272796	15.905547	12.01318
H	14.866766	15.217476	12.206469
C	13.553001	16.494718	13.049302
C	11.908046	14.721046	21.324799
H	12.733573	14.301269	21.416949
C	13.866952	15.971511	14.422558
C	18.733046	12.988454	19.135681
H	17.965259	12.802615	19.625647
C	11.639884	15.493838	20.198774
C	14.124703	16.319385	10.70735
C	12.683612	17.541201	12.743635
C	21.084094	12.815894	18.883954
H	21.908906	12.529221	19.203107
C	12.575422	17.981827	11.440053
H	11.99734	18.683847	11.244516
C	10.428534	16.151449	20.090891
C	13.302337	17.408491	10.424159
H	13.244301	17.741667	9.556602
C	21.003195	13.520042	17.699493
H	21.774642	13.690305	17.209526
C	12.731601	15.503833	19.137928
C	9.45449	16.006484	21.091053
H	8.63115	16.430798	21.010141
U	20.329936	21.394234	16.722481
I	25.446183	21.314373	18.353756
I	17.136072	18.043484	19.854449
I	15.661094	18.952843	15.157509
I	21.273569	21.236221	24.496323
I	25.826453	25.205238	12.600691
Ag	16.559614	19.873986	17.704887
O	22.120851	22.124516	15.236173
O	22.64562	21.974181	17.346627
O	18.096287	20.856061	15.860993
O	20.663134	21.167992	19.140176
O	20.847719	19.716236	16.456595
O	18.736238	20.481972	18.432196
O	19.573569	21.380883	14.364122
O	19.802256	23.044107	16.969038

I	17.061455	23.182933	9.827882
C	24.353338	22.691476	15.816042
C	19.306098	20.139611	20.767405
C	19.561425	20.6184	19.387407
C	18.429076	19.146113	21.156232
C	25.474038	22.479561	16.577963
C	22.970347	22.232184	16.159918
C	24.479373	23.463668	14.674285
H	23.732544	23.62785	14.146109
C	17.351339	21.046175	13.581973
C	20.118967	20.712944	21.751834
H	20.725135	21.378931	21.518089
C	25.70951	23.996131	14.305686
C	17.598555	21.827697	12.451453
H	18.396047	22.302848	12.379531
C	18.372719	18.717299	22.477794
H	17.776264	18.047035	22.72053
C	20.0271	20.295256	23.068901
C	16.159166	20.323515	13.631419
C	26.707821	23.003295	16.213859
H	27.455112	22.85118	16.748777
C	16.663617	21.895893	11.444548
C	18.4007	21.080343	14.660799
C	26.823267	23.745874	15.067607
H	27.652159	24.077227	14.80689
C	19.19196	19.277108	23.435253
H	19.177438	18.967211	24.311799
C	15.246345	20.411735	12.597544
H	14.447865	19.936667	12.644743
C	15.510301	21.191806	11.509728
H	14.896504	21.23838	10.810738
I	14.236183	21.314373	18.353756
I	14.616453	25.205238	12.600691
O	10.910851	22.124516	15.236173
O	11.43562	21.974181	17.346627
C	13.143338	22.691476	15.816042
C	14.264038	22.479561	16.577963
C	11.760347	22.232184	16.159918
C	13.269373	23.463668	14.674285
H	12.522544	23.62785	14.146109
C	14.49951	23.996131	14.305686
C	15.497821	23.003295	16.213859
H	16.245112	22.85118	16.748777

C	15.613267	23.745874	15.067607
H	16.442159	24.077227	14.80689

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