

Supporting Information for

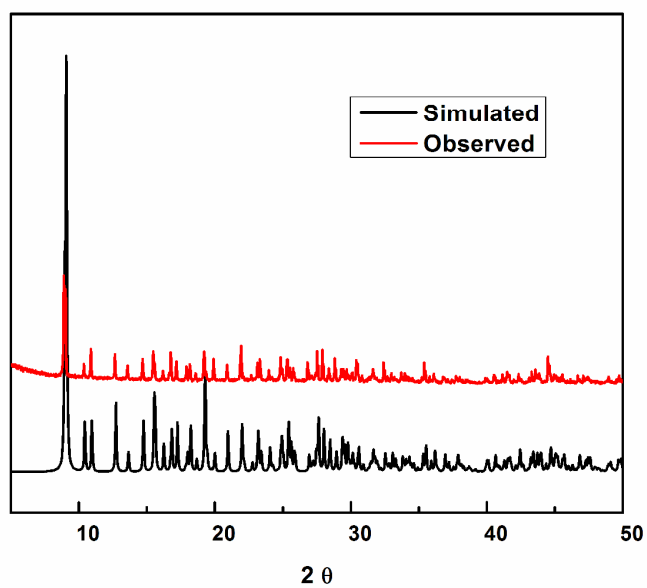
Porous Uranium Diphosphonate Frameworks with Trinuclear Units Templated by Organic Ammonium Hydrolyzed from Amine Solvents

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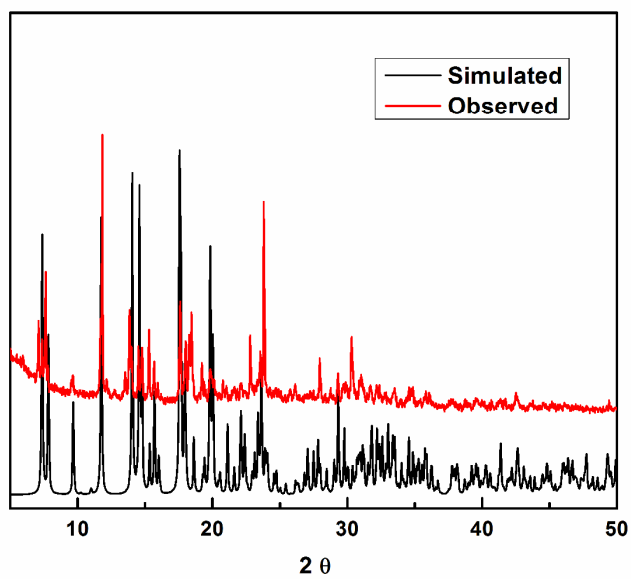
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(a)



(b)

Figure S1. Powder X-ray diffraction (PXRD) patterns of **1** (a) and **2** (b) compared to patterns calculated from the corresponding crystal structure.

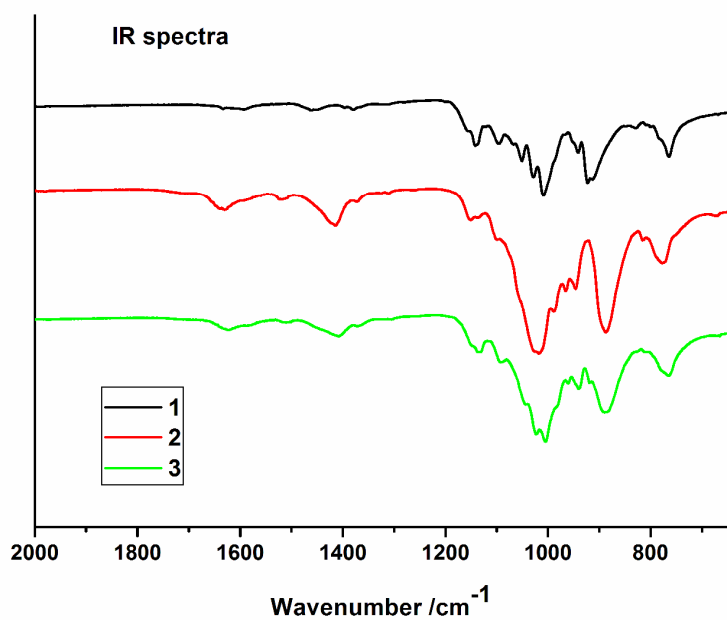


Figure S2. The IR spectra of complexes 1–3 at room temperature.

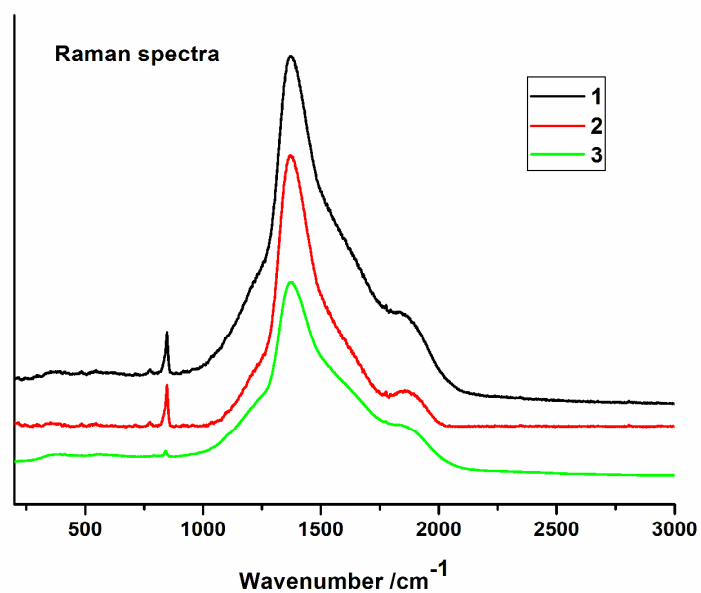


Figure S3. The Raman spectra of complexes 1–3 at room temperature.

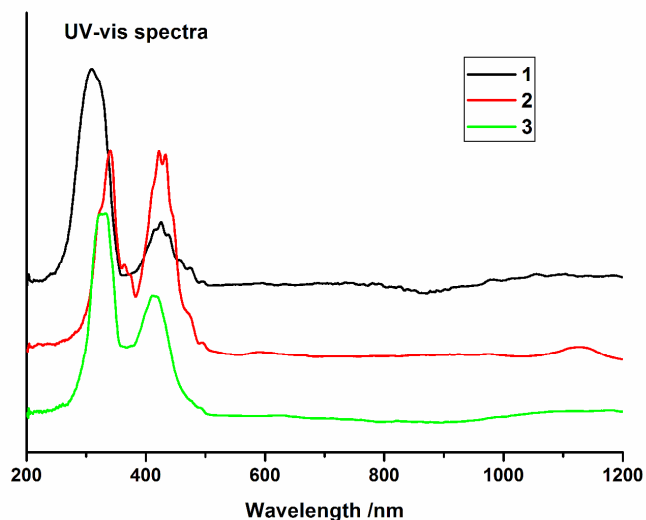


Figure S4. The UV-Vis spectra of complexes **1–3** at room temperature.

Table S1. Selected bond angles (deg) for compounds **1–3**.

Compound 1					
O14—U1—O13	178.5 (3)	O16—U2—O15	178.8 (2)	O17—U3—O18	178.5 (3)
O14—U1—O6 ⁱ	92.5 (2)	O16—U2—O2	91.5 (2)	O17—U3—O5 ⁱⁱⁱ	84.3 (2)
O13—U1—O6 ⁱ	89.0 (2)	O15—U2—O2	89.7 (2)	O18—U3—O5 ⁱⁱⁱ	97.1 (2)
O14—U1—O4	91.5 (2)	O16—U2—O11 ⁱⁱ	88.1 (2)	O17—U3—O12	96.7 (2)
O13—U1—O4	87.1 (2)	O15—U2—O11 ⁱⁱ	92.0 (2)	O18—U3—O12	84.1 (2)
O6 ⁱ —U1—O4	149.00 (18)	O2—U2—O10 ⁱⁱ	126.07 (16)	O7—U2—O8	55.72 (15)
O14—U1—O3 ⁱ	88.0 (2)	O11 ⁱⁱ —U2—O10 ⁱⁱ	57.77 (16)	O1—U2—O8	115.80 (16)
O13—U1—O3 ⁱ	92.1 (2)	O16—U2—O7	88.7 (2)	O5 ⁱⁱⁱ —U3—O12	72.31 (17)
O6 ⁱ —U1—O3 ⁱ	74.70 (18)	O15—U2—O7	91.0 (2)	O17—U3—O9 ⁱⁱ	93.7 (2)
O4—U1—O3 ⁱ	74.73 (18)	O2—U2—O7	117.68 (16)	O18—U3—O9 ⁱⁱ	86.1 (2)
O14—U1—O1	92.0 (2)	O11 ⁱⁱ —U2—O7	173.29 (15)	O5 ⁱⁱⁱ —U3—O9 ⁱⁱ	81.44 (17)
O13—U1—O1	87.1 (2)	O10 ⁱⁱ —U2—O7	116.24 (15)	O12—U3—O9 ⁱⁱ	150.55 (16)
O6 ⁱ —U1—O1	135.10 (17)	O16—U2—O1	91.0 (2)	O17—U3—O10 ⁱⁱ	90.3 (2)
O4—U1—O1	75.40 (17)	O15—U2—O1	89.9 (2)	O18—U3—O10 ⁱⁱ	88.2 (2)
O3 ⁱ —U1—O1	150.12 (17)	O2—U2—O1	57.60 (17)	O5 ⁱⁱⁱ —U3—O10 ⁱⁱ	153.17 (17)
O14—U1—O7	89.6 (2)	O11 ⁱⁱ —U2—O1	125.90 (16)	O12—U3—O10 ⁱⁱ	134.50 (16)
O13—U1—O7	91.2 (2)	O10 ⁱⁱ —U2—O1	176.33 (16)	O9 ⁱⁱ —U3—O10 ⁱⁱ	72.67 (16)
O6 ⁱ —U1—O7	72.69 (17)	O7—U2—O1	60.09 (15)	O17—U3—O8	87.0 (2)
O4—U1—O7	138.10 (18)	O16—U2—O8	87.1 (2)	O18—U3—O8	92.0 (2)
O3 ⁱ —U1—O7	147.15 (17)	O15—U2—O8	91.8 (2)	O5 ⁱⁱⁱ —U3—O8	142.46 (17)
O1—U1—O7	62.70 (16)	O2—U2—O8	173.26 (17)	O12—U3—O8	72.55 (16)
O2—U2—O11 ⁱⁱ	68.35 (17)	O11 ⁱⁱ —U2—O8	118.16 (16)	O9 ⁱⁱ —U3—O8	135.65 (16)
O16—U2—O10 ⁱⁱ	88.9 (2)	O10 ⁱⁱ —U2—O8	60.53 (15)	O10 ⁱⁱ —U3—O8	62.97 (16)

O15—U2—O10 ⁱⁱ	90.1 (2)				
Compound 2					
O1—U1—O7	143.2 (3)	O3—U2—O12	141.9 (3)	O2—U3—O21	72.0 (3)
O4—U1—O1	72.9 (3)	O6—U2—O3	76.3 (2)	O15 ⁱⁱⁱ —U3—O2	71.5 (2)
O4—U1—O5 ⁱ	74.3 (2)	O6—U2—O12	66.6 (3)	O15 ⁱⁱⁱ —U3—O21	142.6 (3)
O4—U1—O7	142.1 (3)	O10—U2—O3	95.2 (3)	O17 ^{iv} —U3—O2	137.7 (2)
O5 ⁱ —U1—O1	146.8 (3)	O10—U2—O6	85.5 (3)	O17 ^{iv} —U3—O15 ⁱⁱⁱ	150.7 (3)
O5 ⁱ —U1—O7	69.8 (3)	O10—U2—O11	179.8 (5)	O17 ^{iv} —U3—O21	66.4 (3)
O8—U1—O1	91.1 (3)	O10—U2—O12	90.5 (4)	O18 ⁱⁱⁱ —U3—O2	145.7 (2)
O8—U1—O4	90.1 (3)	O10—U2—O13 ⁱⁱ	85.7 (3)	O18 ⁱⁱⁱ —U3—O15 ⁱⁱⁱ	74.3 (2)
O8—U1—O5 ⁱ	84.4 (3)	O10—U2—O16 ⁱⁱ	91.6 (3)	O18 ⁱⁱⁱ —U3—O17 ^{iv}	76.4 (3)
O8—U1—O7	98.0 (3)	O11—U2—O3	84.9 (4)	O18 ⁱⁱⁱ —U3—O21	142.2 (3)
O8—U1—O9	179.1 (3)	O11—U2—O6	94.7 (4)	O19—U3—O2	87.2 (3)
O8—U1—O14	88.3 (3)	O11—U2—O12	89.6 (4)	O19—U3—O15 ⁱⁱⁱ	92.1 (3)
O9—U1—O1	89.2 (3)	O11—U2—O13 ⁱⁱ	94.1 (4)	O19—U3—O17 ^{iv}	88.5 (3)
O9—U1—O4	89.1 (3)	O11—U2—O16 ⁱⁱ	88.3 (4)	O19—U3—O18 ⁱⁱⁱ	91.1 (3)
O9—U1—O5 ⁱ	94.8 (3)	O13 ⁱⁱ —U2—O3	75.1 (3)	O19—U3—O20	178.1 (3)
O9—U1—O7	82.2 (3)	O13 ⁱⁱ —U2—O6	149.1 (2)	O19—U3—O21	94.2 (3)
O9—U1—O14	92.7 (3)	O13 ⁱⁱ —U2—O12	143.0 (3)	O20—U3—O2	91.2 (3)
O14—U1—O1	71.4 (3)	O16 ⁱⁱ —U2—O3	150.7 (2)	O20—U3—O15 ⁱⁱⁱ	88.2 (3)
O14—U1—O4	144.2 (2)	O16 ⁱⁱ —U2—O6	132.7 (2)	O20—U3—O17 ^{iv}	92.1 (3)
O14—U1—O5 ⁱ	140.9 (2)	O16 ⁱⁱ —U2—O12	66.2 (3)	O20—U3—O18 ⁱⁱⁱ	90.8 (3)
O14—U1—O7	73.3 (3)	O16 ⁱⁱ —U2—O13 ⁱⁱ	77.0 (3)	O20—U3—O21	84.5 (3)
Compound 3					
O9—U1—O8	178.98 (18)	O5 ⁱ —U1—O1	76.05 (13)	O5 ⁱ —U1—O7	142.07 (12)
O9—U1—O3 ⁱ	91.40 (16)	O9—U1—O4	87.09 (15)	O1—U1—O7	141.87 (12)
O8—U1—O3 ⁱ	89.62 (16)	O8—U1—O4	92.20 (16)	O4—U1—O7	66.14 (12)
O9—U1—O5 ⁱ	86.80 (15)	O3 ⁱ —U1—O4	130.54 (12)	O12—U2—O2 ⁱⁱⁱ	89.75 (16)
O8—U1—O5 ⁱ	93.48 (15)	O5 ⁱ —U1—O4	151.08 (13)	O12—U2—O6 ⁱⁱ	89.49 (15)
O3 ⁱ —U1—O5 ⁱ	77.86 (13)	O1—U1—O4	75.93 (13)	O2 ⁱⁱⁱ —U2—O6	86.33 (13)
O9—U1—O1	91.93 (15)	O9—U1—O7	90.03 (15)	O10—Na1—O11 ^v	91.5 (2)
O8—U1—O1	87.19 (15)	O8—U1—O7	90.35 (15)	O10—Na1—O9 ^v	88.2 (2)
O3 ⁱ —U1—O1	153.46 (13)	O3 ⁱ —U1—O7	64.43 (12)	O11—Na1—O9 ^v	101.22 (15)

Symmetry codes: **1**, (i) $-x + 2, -y + 3/2, z + 1/2$; (ii) $x - 1/4, -y + 5/4, z - 1/4$; (iii) $-x + 7/4, y - 1/4, z + 1/4$. **2**, (i) $-x, -y + 2, -z$; (ii) $-x, -y + 1, -z$; (iii) $x + 1, y, z$; (iv) $-x, -y + 1, -z + 1$. **3**, (i) $-x, y - 1/2, -z + 1/2$; (ii) $-x + 1, -y, -z + 1$; (iii) $x + 1, y, z$; (v) $-x, -y, -z$.