Supporting Information. Tables S1-S5 and Figures S1-S6. This material is available free of charge via the Internet at http://pubs.acs.org.

Table S1. Crystal data and structure refinement for Compound 1.

Identification code	Compound1	
Empirical formula	C66 H42 In2 N4 O13	
Formula weight	1328.66	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.835(2) Å	α= 96.492(4)°.
	b = 13.839(3) Å	β= 100.320(5)°.
	c = 21.881(5) Å	γ= 104.967(4)°.
Volume	2790.5(11) Å3	
Z	2	
Density (calculated)	1.579 Mg/m3	
Absorption coefficient	0.899 mm-1	
F(000)	1332	
Crystal size	0.30 x 0.25 x 0.20 mm3	
Theta range for data collection	0.96 to 20.81°.	
Index ranges	-9<=h<=9, -13<=k<=13, -21<=l<=21	
Reflections collected	12374	
Independent reflections	5647 [R(int) = 0.1929]	
Completeness to theta = 20.81°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.835 and 0.764	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	5647 / 0 / 775	
Goodness-of-fit on F2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0758, wR2 = 0.1700	
R indices (all data)	R1 = 0.1252, wR2 = 0.2108	
Largest diff. peak and hole	1.094 and -0.964 e.Å-3	

Table S2. Crystal data and structure refinement for Compound 2.

Identification code	Compound2	
Empirical formula	C19 H13.5 In N O5.25	
Formula weight	454.38	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.7789(3) Å	α= 90°.
	b = 8.2923(2) Å	β= 95.0310(10)°.
	c = 19.6538(5) Å	γ = 90°.
Volume	1749.93(8) Å3	
Z	4	
Density (calculated)	1.725 Mg/m3	
Absorption coefficient	11.083 mm-1	
F(000)	901	
Crystal size	0.08 x 0.04 x 0.04 mm3	
Theta range for data collection	4.52 to 63.28°.	
Index ranges	-12<=h<=12, -9<=k<=9, -22<=l<=18	
Reflections collected	22655	
Independent reflections	2832 [R(int) = 0.0361]	
Completeness to theta = 63.28°	99.1 %	
Absorption correction	None	
Max. and min. transmission	0.6655 and 0.4709	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2832 / 1 / 230	
Goodness-of-fit on F2	1.065	
Final R indices [I>2sigma(I)]	R1 = 0.0739, wR2 = 0.2276	
R indices (all data)	R1 = 0.0918, wR2 = 0.2452	
Largest diff. peak and hole	1.686 and -1.126 e.Å-3	

Table S3. Crystal data and structure refinement for Compound 3.

Identification code	incompound3
Empirical formula	C38 H27 In N2 O9
Formula weight	770.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 12.8039(9) Å α= 90°.
	b = 14.0375(9) Å β= 90°.
	c = 18.3577(12) Å γ = 90°.
Volume	3299.5(4) Å3
Z	4
Density (calculated)	1.551 Mg/m3
Absorption coefficient	0.778 mm-1
F(000)	1560
Crystal size	0.40 x 0.30 x 0.20 mm3
Theta range for data collection	1.83 to 28.32°.
Index ranges	-16<=h<=16, -18<=k<=18, -24<=l<=24
Reflections collected	30563
Independent reflections	8003 [R(int) = 0.0594]
Completeness to theta = 28.32°	98.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	8003 / 2 / 559
Goodness-of-fit on F2	1.073
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0621
R indices (all data)	R1 = 0.0519, wR2 = 0.0646
Absolute structure parameter	0.002(15)
Largest diff. peak and hole	0.764 and -0.395 e.Å-3

Table S4. Crystal data and structure refinement for Compound 4.

Identification code	InCompound4	
Empirical formula	C76 H54 In2 N4 O18	
Formula weight	1540.87	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9495(6) Å	α= 82.5430(10)°.
	b = 13.0898(8) Å	β= 85.4720(10)°.
	c = 13.2297(8) Å	γ= 80.5710(10)°.
Volume	1682.4(12) Å3	
Z	1	
Density (calculated)	1.521 Mg/m3	
Absorption coefficient	0.763 mm-1	
F(000)	780	
Crystal size	0.30 x 0.25 x 0.20 mm3	
Theta range for data collection	1.59 to 26.37°.	
Index ranges	-12<=h<=12, -16<=k<=16, -16<=l<=16	
Reflections collected	13615	
Independent reflections	6578 [R(int) = 0.0425]	
Completeness to theta = 26.37°	95.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8624 and 0.8035	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	6578 / 2 / 460	
Goodness-of-fit on F2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0860	
R indices (all data)	R1 = 0.0610, wR2 = 0.0922	
Largest diff. peak and hole	0.643 and -0.435 e.Å-3	

Table S5. Crystal data and structure refinement for Compound 5.

Identification code	Incompound5
Empirical formula	C76 H50 In2 N4 O16
Formula weight	1504.84
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.6135(12) Å α= 75.745(2)°.
	b = 11.6513(13) Å β= 68.609(2)°.
	c = 14.0949(15) Å γ= 88.736(2)°.
Volume	1568.5(3) Å3
Z	1
Density (calculated)	1.593 Mg/m3
Absorption coefficient	0.814 mm-1
F(000)	760
Crystal size	0.30 x 0.25 x 0.20 mm3
Theta range for data collection	1.81 to 28.85°.
Index ranges	-13<=h<=13, -15<=k<=15, -18<=l<=18
Reflections collected	13544
Independent reflections	7022 [R(int) = 0.0527]
Completeness to theta = 28.85°	85.3 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	7022 / 0 / 542
Goodness-of-fit on F2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0652, wR2 = 0.0979
R indices (all data)	R1 = 0.1009, wR2 = 0.1072

Largest diff. peak and hole 0.994 and -0.831 e.Å-3

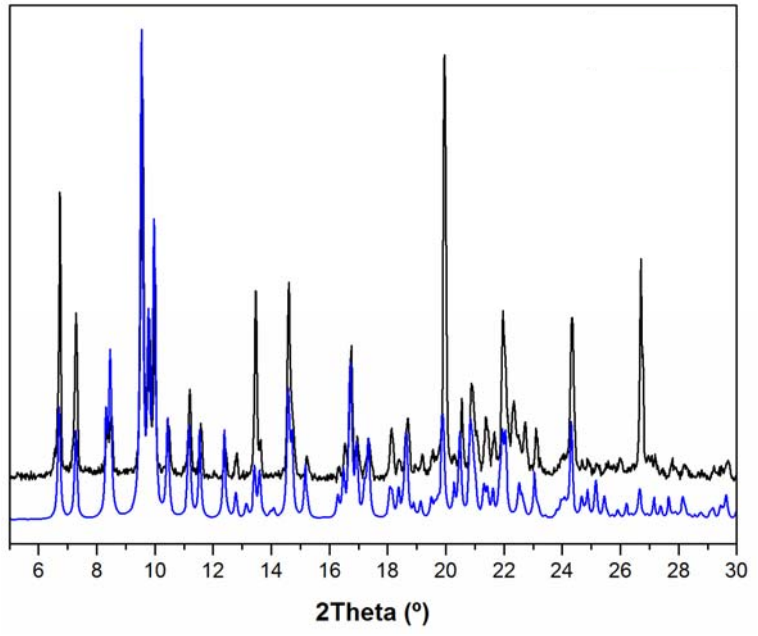

Figure S1. Comparison of the experimental PXRD patterns for as-synthesized compound **1** (black) with the simulated pattern from single-crystal X-Ray data (blue).

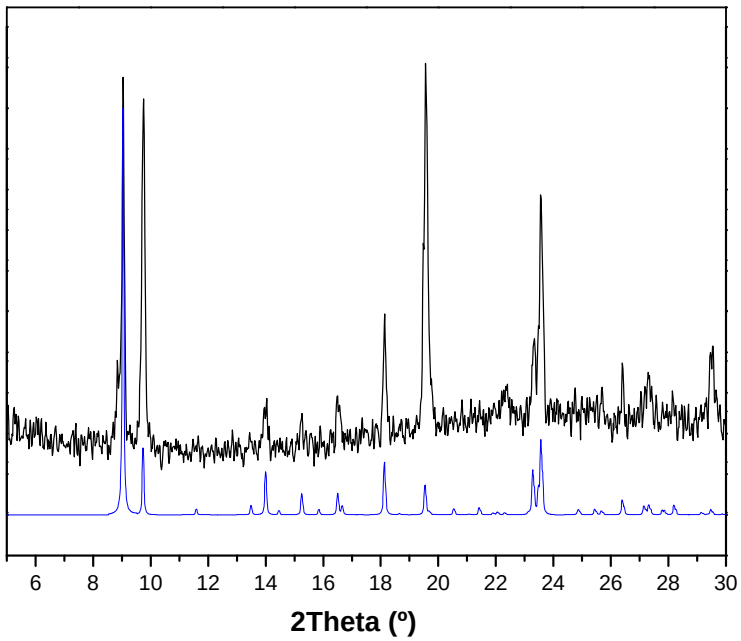

Figure S2. Comparison of the experimental PXRD patterns for as-synthesized compound **2** (black) with the simulated pattern from single-crystal X-Ray data (blue).

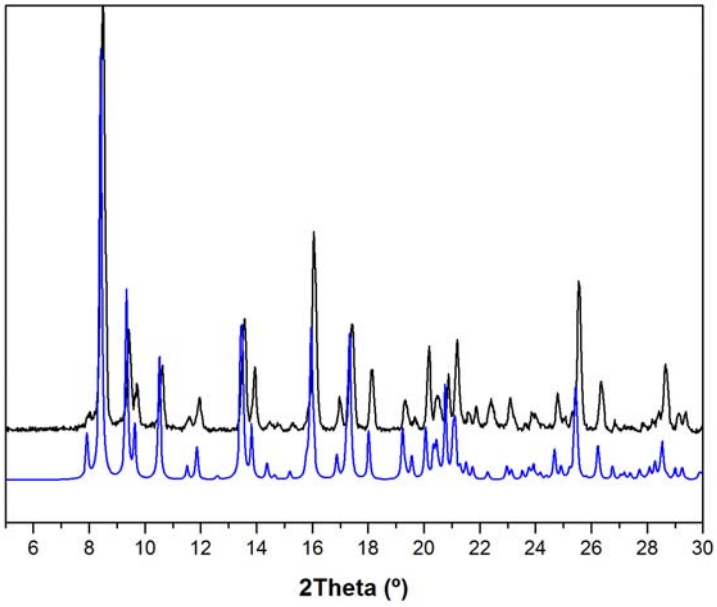

Figure S3. Comparison of the experimental PXRD patterns for as-synthesized compound **3** (black) with the simulated pattern from single-crystal X-Ray data (blue).

TGA curves for **1-3** are shown in **Figure S4**, which reveal the thermal stability of these compounds up to ~300 ºC (under N_2). In order to check their structural stability after losing water molecules, XRPD patterns of the samples heated at 250ºC were recorded (**Figure S5-S7**).

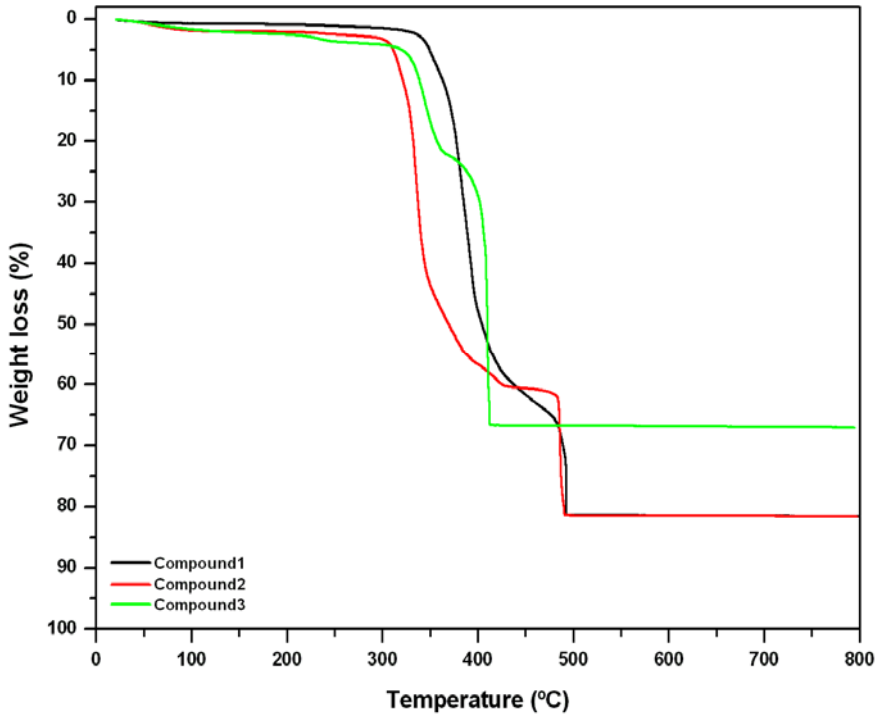

Figure S4. TGA profiles of **1**, **2** and **3** compounds performed under N_2 (flow of 50 mL.min^{-1}) with a heating rate of 5 ºC/min.

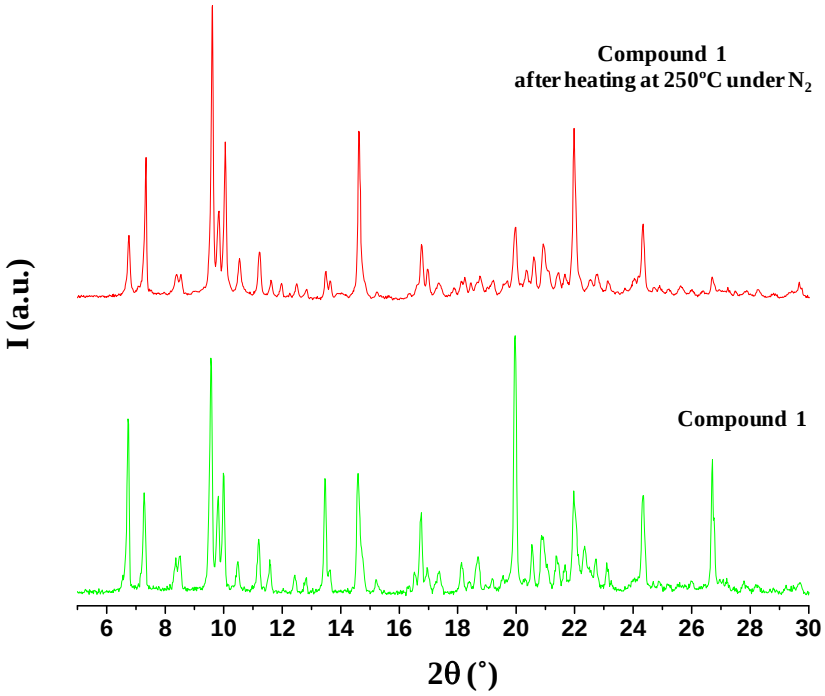

Figure S5. Comparison of the experimental XRPD pattern of **1** after heating a 250ºC under N_2, with the pattern of the as-synthesized sample.

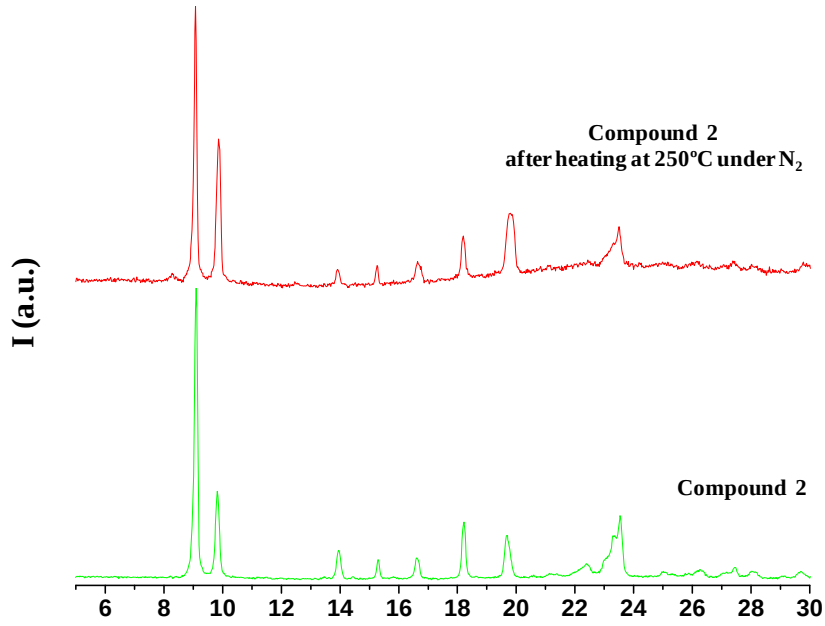

Figure S6. Comparison of the experimental XRPD pattern of **2** after heating a 250ºC under N_2, with the pattern of the as-synthesized sample.

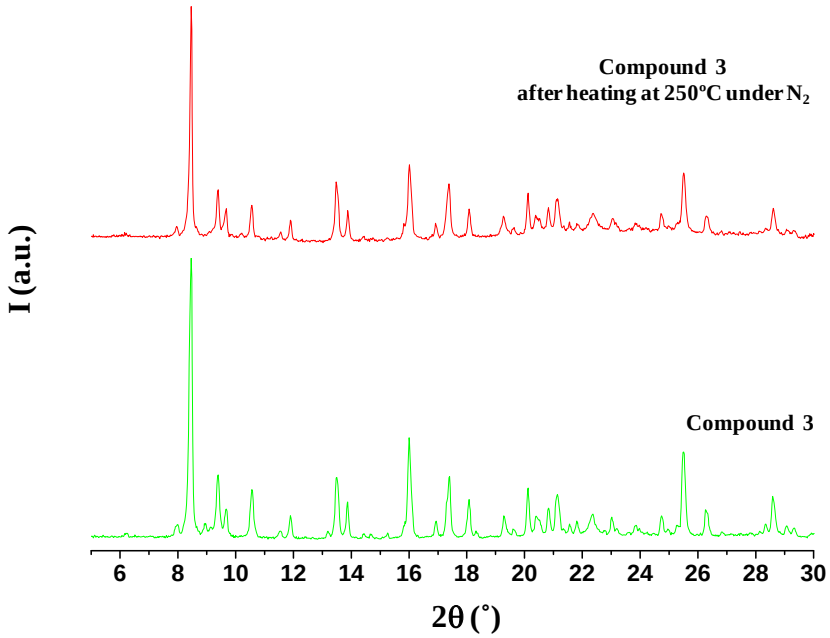

Figure S7. Comparison of the experimental XRPD pattern of **3** after heating a 250ºC under N_2, with the pattern of the as-synthesized sample.

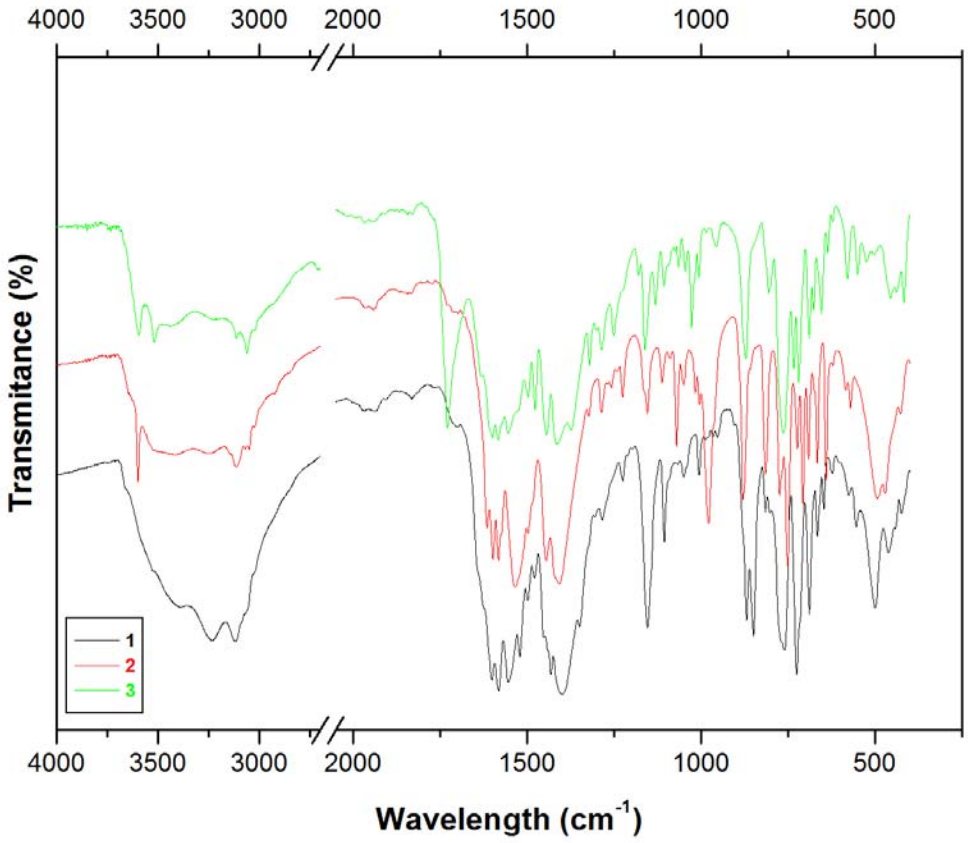

Figure S8. FTIR spectra of compounds 1-**3** in the 4000-250 cm^{-1} range.