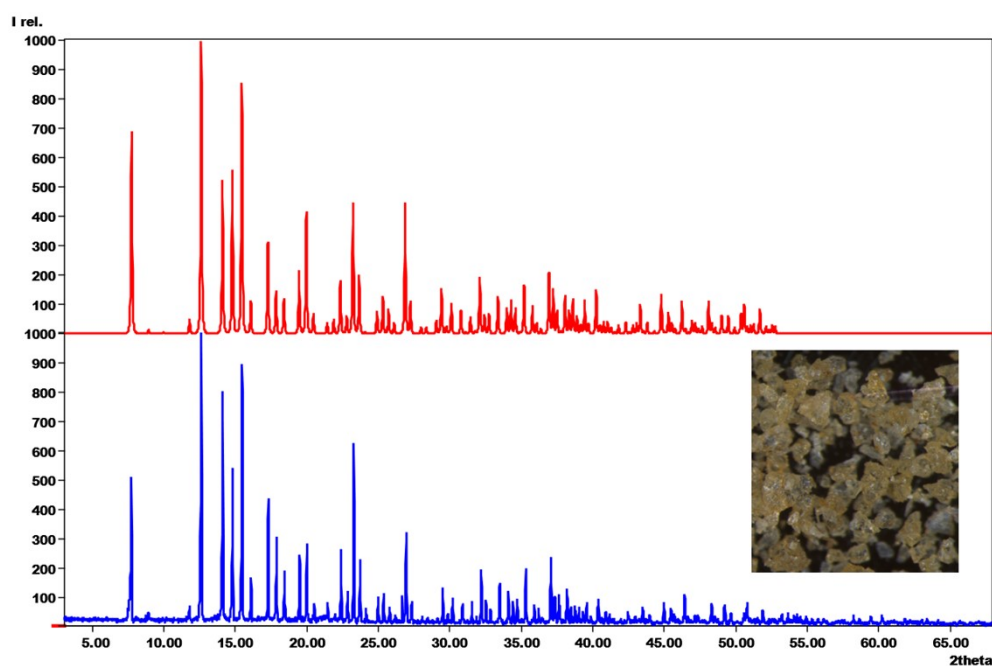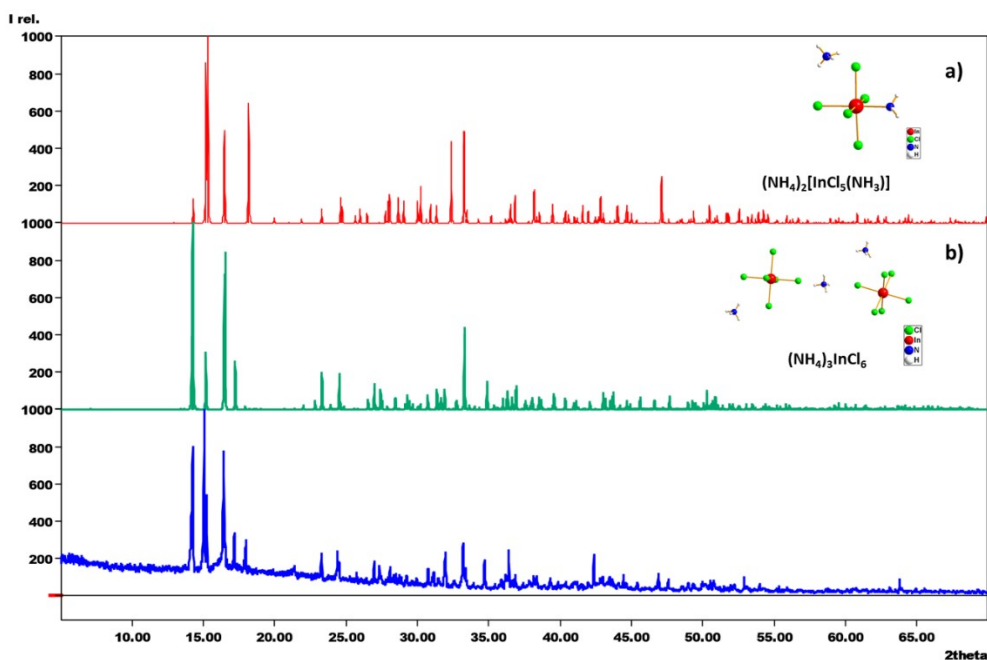# Thermal Deprotonation and Condensation of Melamine in the Presence of Indium(III)chloride

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Supporting Information

Figure SI 1. XRD pattern of the synthesized $(NH_4)[(InCl_2)_3 (C_{12}N_{20}H_8)]\cdot\frac{2}{3}[InCl_3(NH_3)]$(bottom), Calculated pattern from single crystal measurement (top) (CCDC code: 2333063).

Figure SI.2. XRD pattern of the side-phases sublimated on the top part of ampule synthesized along with the main phase of $(NH_4)[(InCl_2)_3 (C_{12}N_{20}H_8)]\cdot\frac{2}{3}[InCl_3(NH_3)]$ (bottom). **(a)** Calculated pattern from single crystal measurement of $(NH_4)_2[InCl_5(NH_3)]$ (CCDC code: 2301094) **(b)** Calculated pattern from single crystal measurement of $(NH_4)_3 InCl_6$ (CCDC code: 2334831).
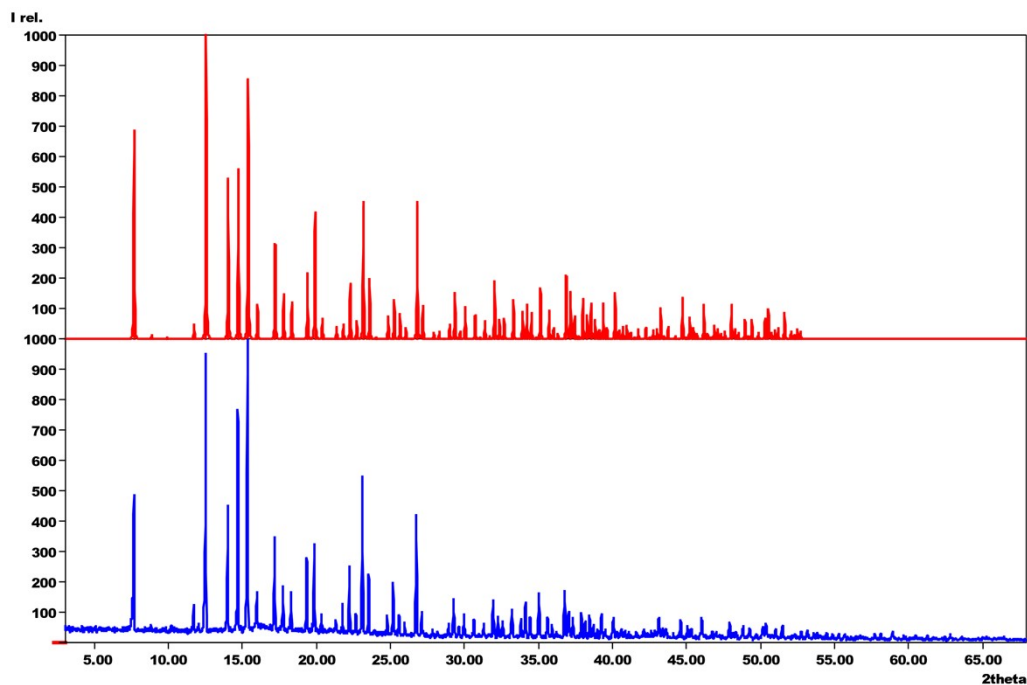
Table S1. Crystal structure data of $(NH_4)_2[InCl_5(NH_3)]$, and $(NH_4)_3 InCl_6$ as side phases of the reaction.

| Empirical Formula	$(NH_4)_2[InCl_5(NH_3)]$		$(NH_4)_3 InCl_6$	
CCDC code	2301094		2334831	
Formula weight (g/mol)	345.19		381.65	
Wavelength (Cu-Kα) (Å)	1.54184		1.54184	
Crystal system	orthorhombic		monoclinic	
Space group	*Pnma*		*P2$_1$/c*	
Unit cell dimensions (Å)	a/Å	13.7070(2)	a/Å	13.1270(3)
	b/Å	10.76210(10)	b/Å	7.78800(10)
	c/Å	6.93960(10)	c/Å	12.2894(2)
Volume (Å³)	1023.70(2)		1192.96(4)	
Z	4		4	
Density (calculated) (g/cm³)	2.240		2.125	
Absorption coefficient (mm⁻¹)	29.980		27.819	
Final R indices (I>2σ(I)) a)	$R_1 = 0.0133$, $wR_2 = 0.0364$		$R_1 = 0.0148$, $wR_2 = 0.0371$	

		R indices (all data)	R$_1$ = 0.0133, wR$_2$ = 0.0364	R$_1$ = 0.0149, wR$_2$ =0.0372
		GOOF	1.264	1.211

Table S2. Vibrational frequencies (in cm^{-1}) for In-Ring compared to those of Melamine, Melem, and $(NH_4)[(InCl_2)_3 (C_{12}N_{20}H_8)]\cdot\frac{2}{3}[InCl_3(NH_3)]$

	Melamine	Melem	$(NH_4)[(InCl_2)_3(C_{12}N_{20}H_8)]\cdot\frac{2}{3}[InCl_3(NH_3)]$
Ring-sextant out-of-plane bending	813	804	792
CNC bending	1193	1306	1284
Side-chain CN breathing	1434 1440 1550	1470	1380 1434 1504
NH$_2$ bending	1652	1612	1647
NH stretching	3128 3334 3421 3469	3119 3325 3424 3487	3200 3348 3452

Figure SI 3. XRD pattern of the synthezied $(NH_4)[(InCl_2)_3 (C_{12}N_{20}H_8)]\cdot\frac{2}{3}[InCl_3(NH_3)]$ after two month in ambient condition(bottom), Calculated pattern from single crystal measurement (top) (CCDC code: 2333063).
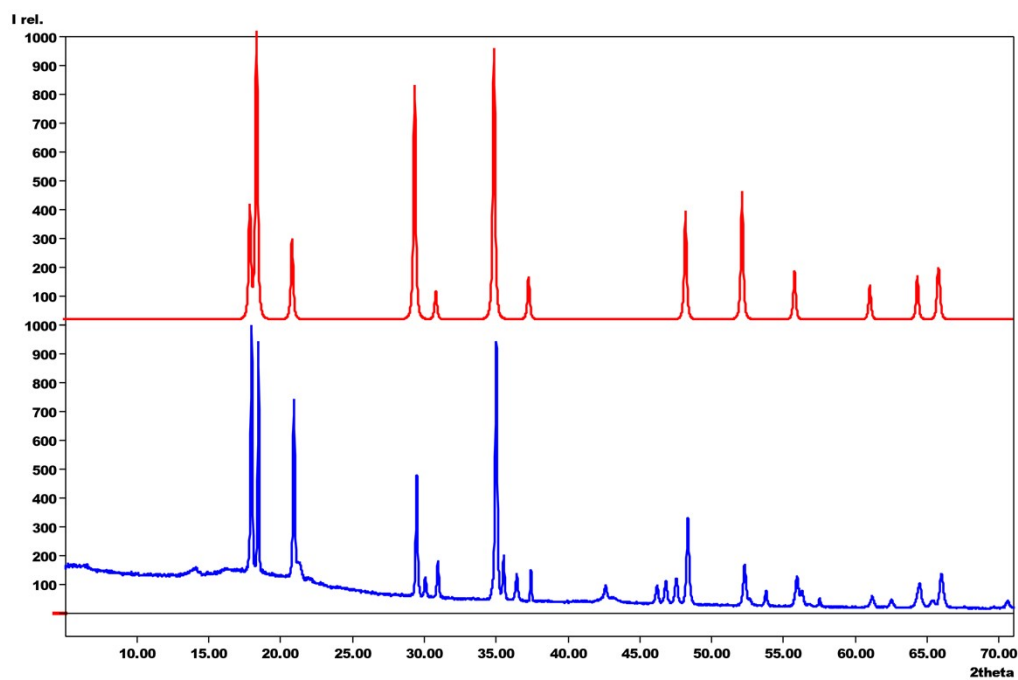
Figure SI 4. The XRD pattern taken from decomposed material at 700˚C in TGA analysis(bottom), Calculated pattern from single crystal measurement of $In_{2.24}(NCN)_3$(top)