Supplementary Information

Ammonium affects the wet chemical network of the HCN: Feedback between prebiotic chemistry and materials science

Cristina Pérez-Fernández, Jorge Vega, José L. de la Fuente, Eva Mateo-Martí, Pilar Valles, and Marta Ruiz-Bermejo*

* Corresponding author. E-mail: ruizbm@cab.inta-csic.es

This PDF file includes:

- Tables S1 and S2
- A comparative study by XPS (Figures S1 and S2)
- Morphological analysis by SEM (Figure S3)

Table S1. Kinetic parameters of a empirical model and initial pH values for each of the polymerization reactions at 90 °C with different ammonium concentration. *pH was adjusted with HCl until pH = 9.2 for a null initial concentration of NH_4^+ .

[NH4 ⁺] (M)	рH	Vmax	k	n	R ²	
0	9.2*	19.8	50.5	2.7	0.99	
0.25	9.8	9.6	64.3	1.6	0.97	
0.50	9.6	22.0	97.6	1.6	0.99	
0.75	9.4	30.4	124.7	1.4	0.99	
1	9.2	35.7	129.1	1.4	0.99	

Table S2. Characteristic parameters for the thermal decomposition of cyanide polymers at different initial ammonium concentrations, showing the main stages observed in the samples: drying stage (<150 °C), main pyrolysis stage (150-450 °C) and carbonization (> 450 °C). ML = Mass loss.

[NH ₄ +] (M)	Stage I, 25-150 °C			Stage II, 150-450 °C			Stage III, 450-1000 °C		
	ML (%)	T _{pmax.} (°C)	dW/dT (%/°C)	ML (%)	T _{pmax.} (°C)	dW/dT (%/°C)	ML (%)	T _{pmax.} (°C)	dW/dT (%/°C)
0	8	86	0.09	23	292 397	0.09 0.09	52	653 787	0.13 0.11
0.25	9	88	0.10	22	292 412	0.09 0.08	52	657 790	0.14 0.12
0.50	8	86	0.09	19	298 418	0.07 0.08	51	658 807	0.13 0.10
0.75	8	88	0.10	19	268 408	0.06	52	653 812	0.14 0.10
1	9	77	0.11	16	417	0.08	51	667 827	0.14 0.09



Figure S1. XPS photoemission spectra of the C1s, N1s, and O1s core level peaks of cyanide polymers synthetized at the same initial pH value of 9.2 [adjusting with HCl, $[NH_4^+] = 0$ M (red spectra) and adjusting with NH₄Cl 1 M (black spectra)].



Figure S2. XPS photoemision spectra of the C 1s (a-b), N 1s (c-d) and O 1s (e-f) core level peaks of cyanide polymers synthetized at the same initial pH value of 9.2 (adjusting with HCI, $[NH_4^+] = 0$ M, or with NH₄Cl 1 M). Experimental core-level spectra (black), the result of a fitting of several components (red) and components (black dotted line). Very similar XPS spectra were recorded for the samples synthetized using ammonium concentrations of 0.25, 0.5 and 0.75 M.

Morphological analysis by SEM



Figure S3. SEM images for cyanide polymers at different initial ammonium concentrations: a-c) 0 M (pH = 9.2); d-f) 0.25 M; g-i) 0.5 M; j-l) 0.75 M; and m-o) 1 M.