Supplementary Information

Molecular self-assembly of 1D infinite polyiodide helices in a phenanthrolinium salt

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1. Crystallographic data for **phenpi**

Electronic Supplementary Information (ESI) available: CCDC 2041514 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table .1. Selected crystallographic data for **phenpi**

Empirical formula	$C_{72}H_{51}I_7N_{12}$
Formula weight	1972.55
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$Pna2_1$
***a*/Å**	24.0054(3)
***b*/Å**	12.4116(2)
***c*/Å**	22.5277(5)
***α*/°**	90
***β*/°**	90
***γ*/°**	90
Volume/Å³	6712.0(2)
Z	4
ρ_{calc}**g/cm³**	1.952
μ**/mm⁻¹**	25.833
F(000)	3752.0
Crystal size/mm³	0.793 × 0.128 × 0.084
Radiation	Cu$K\alpha$ (λ = 1.54184)
2ϑ range for data collection/°	7.85 to 136.496
Index ranges	-28 ≤ h ≤ 28, -14 ≤ k ≤ 14, -18 ≤ l ≤ 27
Reflections collected	32490
Independent reflections	9745 [R_{int} = 0.0580, R_{sigma} = 0.0472]
Data/restraints/parameters	9745/39/424
Goodness-of-fit on F^2	1.172
Final R indexes [I>=2σ (I)]	R_1 = 0.0578, wR_2 = 0.1392
Final R indexes [all data]	R_1 = 0.0624, wR_2 = 0.1417
Largest diff. peak/hole / e Å⁻³	1.25/-2.40
Flack parameter	0.012(8)

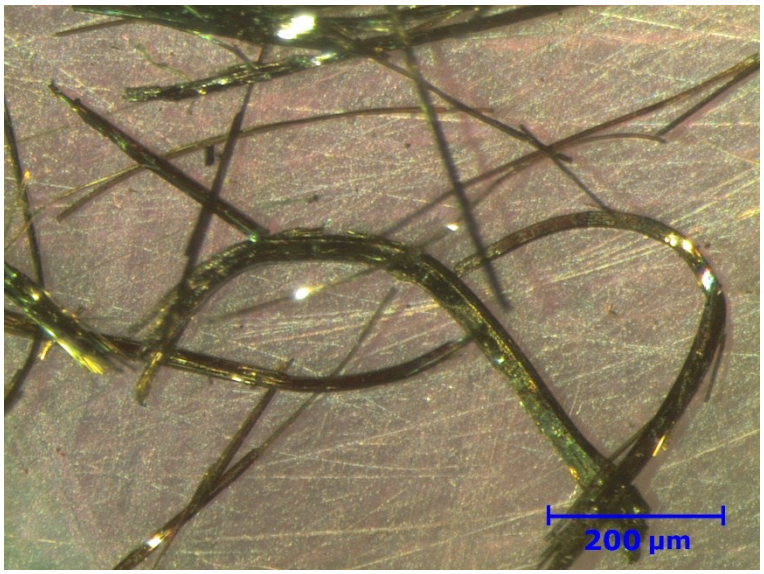

Figure 1. Microphotograph of **phenpi** crystals.

2. Powder diffraction data for **phenpi**

Powder diffraction data was fitted using Pawley method, as implemented in TOPAS software. Refined unit cell parameters at 298 K are: *a* = 23.8503(5) Å, *b* = 12.5979(4) Å, *c* = 22.2769(7) Å, α=β=γ= 90° (Figure 2 SI; Rwp =3.35%,

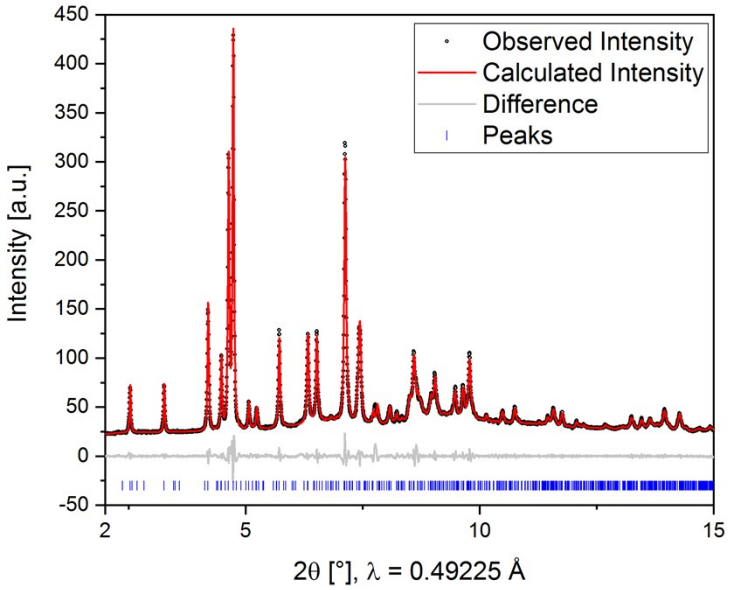

Figure 2. PXRD data for **phenpi.**

GoF = 2.46).

3. Mass spectra for decomposition products of **phenpi**

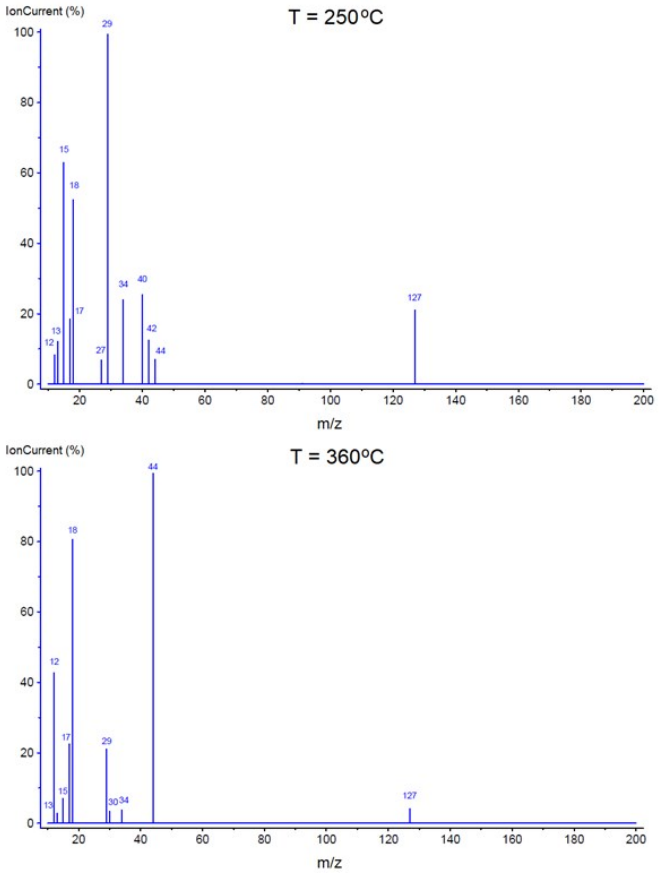

Figure 3. Mass spectra of volatile products from the thermal decomposition of phenpi registered at 250°C and 360°C. The elaboration of the mass spectra involved subtracting the background spectrum and application of an automatic software correction for the carrier gas.