Electronic Supporting Information

Development of transition metal-free polymerization route to functional conjugated polydiynes from haloalkyne-based organic reaction

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Table S1 Crystal data and structure refinement for model compound **7**.

Empirical formula	$C_{56}H_{37}\cdot CHCl_3$	
Formula weight	829.22	
Temperature	100.0(5) K	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.65924(8) Å	α= 90°.
	b = 9.12014(9) Å	β= 91.6555(9)°.
	c = 50.6162(5) Å	γ = 90°.
Volume	4457.10(7) Å^3	
Z	4	
Density (calculated)	1.236 g/cm^3	
μ/mm^{-1}	2.142	
F(000)	1724.0	
Crystal size/mm^3	0.25 × 0.2 × 0.08	
Radiation	CuKα (λ = 1.54184)	
2Θ range for data collection/°	9.71 to 133.992	
Index ranges	$-9 \le h \le 11$, $-10 \le k \le 7$, $-60 \le l \le 60$	
Reflections collected	18636	
Independent reflections	7798 [R_{int} = 0.0181, R_{sigma} = 0.0243]	
Data/restraints/parameters	7798/0/553	
Completeness to theta = 66.5°	98.1%	
Goodness-of-fit on F^2	1.002	
Final R indexes [I>=2σ (I)]	R_1 = 0.0895, wR_2 = 0.2148	
Final R indexes [all data]	R_1 = 0.0973, wR_2 = 0.2209	
Largest diff. peak/hole / e Å^{-3}	1.47/-1.10	