Electronic Supplementary Information (ESI)

Cu(I)-Catalyzed Amino-Yne Click Polymerization

Benzhao He,† Shijie Zhen,† Yongwei Wu,† Rongrong Hu,† Zujin Zhao,† Anjun Qin,,† and Ben Zhong Tang*,†,‡*

† Guangdong Innovative Research Team, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, China.

‡ Department of Chemistry, Hong Kong Branch of Chinese National Engineering Research Center for Tissue Restoration and Reconstruction, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong, China.

Table of contents

solvent peaks are marked with asterisks. S7

Table S1. Crystal data and structure refinement of monomer 1

Empirical formula	$C_{33}H_{24}O_4$	
Formula weight	484.52	
Temperature	293 K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.8102(8) Å	α = 105.048(8)°.
	b = 12.1290(11) Å	β = 91.812(7)°.
	c = 13.7804(11) Å	γ = 110.568(8)°.
Volume	1319.1(2) Å^3	
Z	2	
Density (calculated)	1.220 mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	508	
Crystal size	0.45 × 0.36 × 0.28 mm^3	
Theta range for data collection	3.11 to 25.35°.	
Index ranges	-10<=h<=8, -14<=k<=13, -14<=l<=16	
Reflections collections	8271	
Independent reflections	4828 [R(int) = 0.0256]	
Completeness to theta = 66.50°	99.57%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.88392	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4828 / 0 / 337	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1227	
R indices (all data)	R1 = 0.0865, wR2 = 0.1478	
Largest diff. peak and hole	0.325 and -0.304 e.Å^{-3}	

Table S2. Crystal data and structure refinement of model compound 4.

Empirical formula	$C_{45}H_{38}N_2O_4$	
Formula weight	670.77	
Temperature	293 K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 12.0454(6) Å	$\alpha = 90.00^o$.
	b = 19.9342(12) Å	$\beta = 90.00^o$.
	c = 15.6271(7) Å	$\gamma = 90.00^o$.
Volume	3752.3(3) $Å^3$	
Z	4	
Density (calculated)	1.187 mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	1416	
Crystal size	0.40 × 0.30 × 0.26 mm^3	
Theta range for data collection	2.96 to 25.35°.	
Index ranges	-14<=h<=12, -21<=k<=24, -18<=l<=17	
Reflections collections	22198	
Independent reflections	3433 [R(int) = 0.0473]	
Completeness to theta = 66.50°	99.65%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.95672	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3433 / 0 / 232	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1089	
R indices (all data)	R1 = 0.0777, wR2 = 0.1261	
Largest diff. peak and hole	0.154 and -0.129 $e.Å^{-3}$	

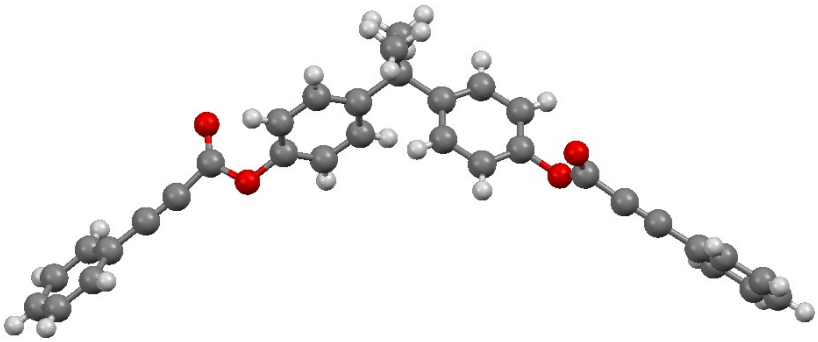

Figure S1. Single crystal structure (CCDC 1457164) of monomer **1**.

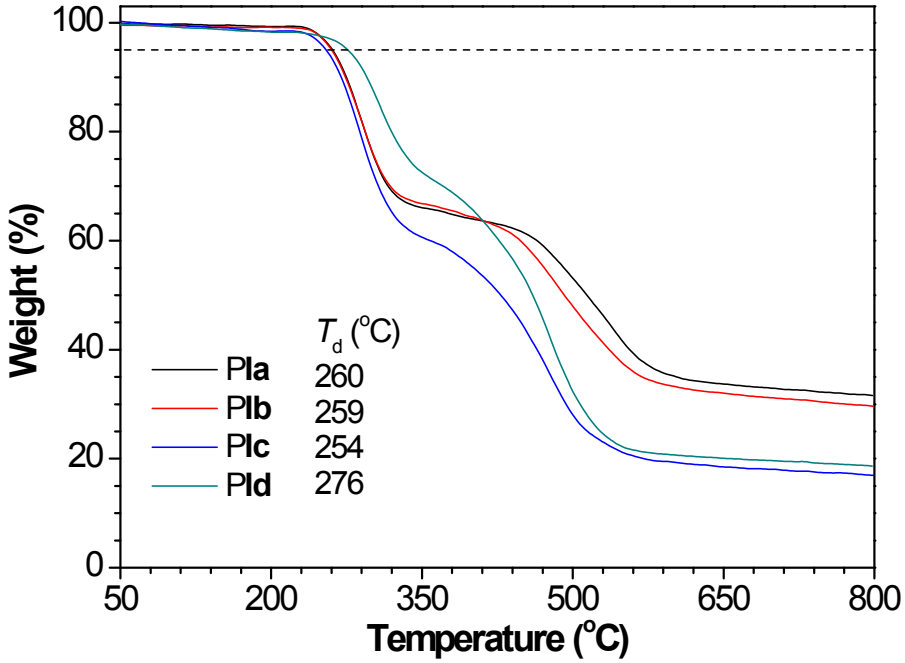

Figure S2. TGA curves of P**Ia**-P**Id** recorded under nitrogen at a heating rate of 10 °C/min.

Table S3. The weight loss in the first decomposition stage.

polymers	experimental values (%)	calculated values (%)
P**Ia**	34.2	33.1
P**Ib**	33.3	33.0
P**Ic**	39.5	38.0

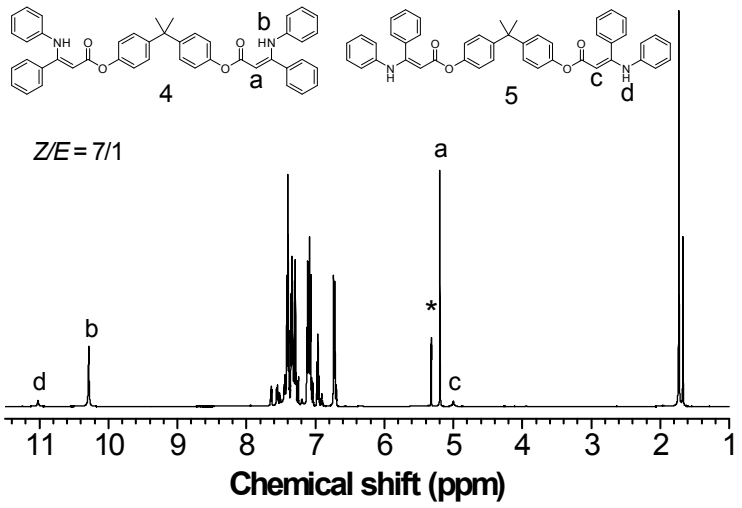

Figure S3 ^{1}H NMR spectra of crude product of model reaction in dichloromethane-d_2. The solvent peaks are marked with asterisks.

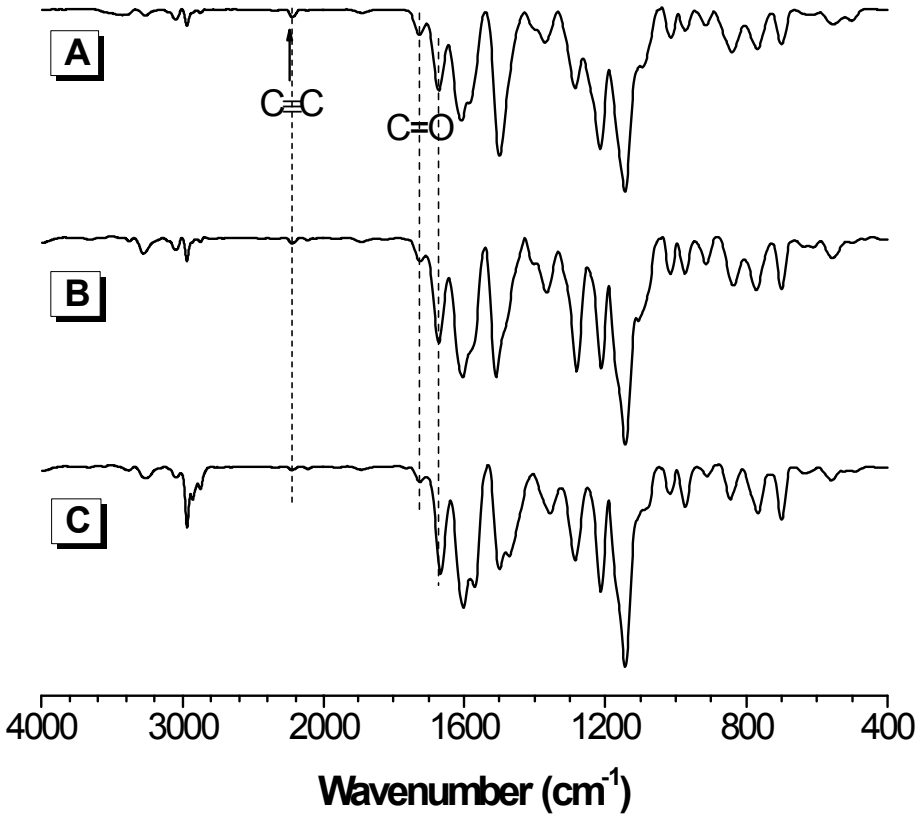

Figure S4. FT-IR spectra of (A) P**Ib**, (B) P**Ic** and (C) P**Id**.

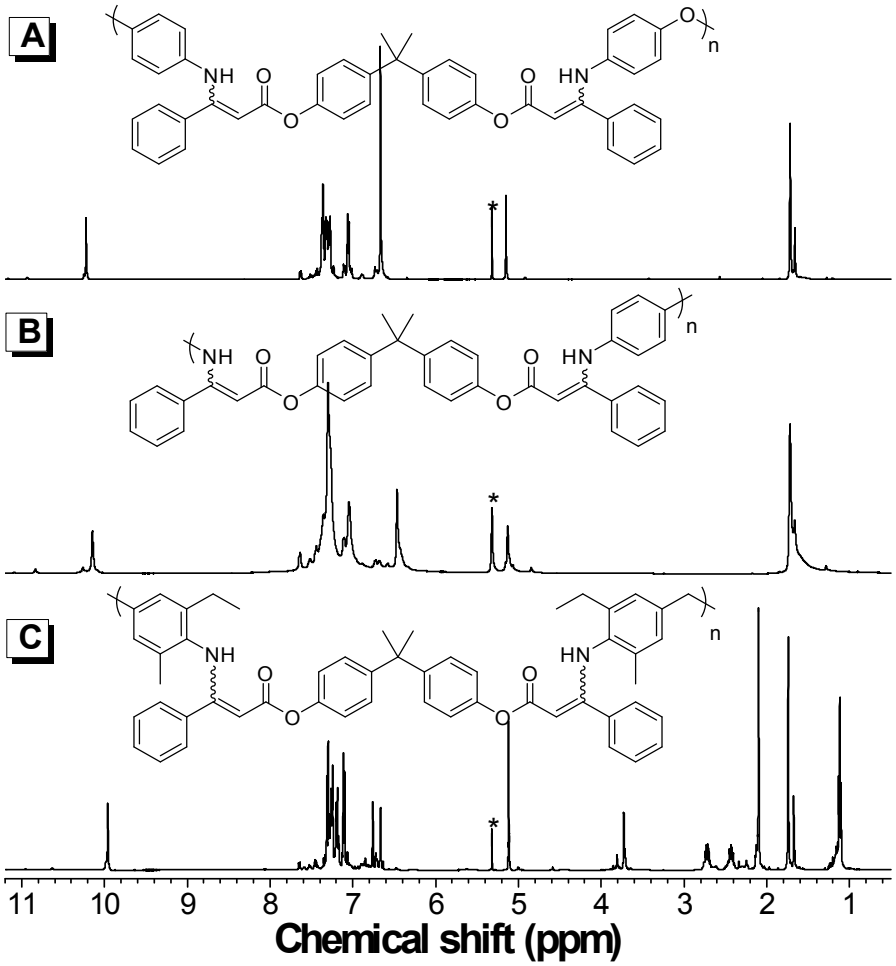

Figure S5. ^{1}H NMR spectra of (A) P**Ib**, (B) P**Ic** and (C) P**Id** in dichloromethane-d_2. The solvent peaks are marked with asterisks.

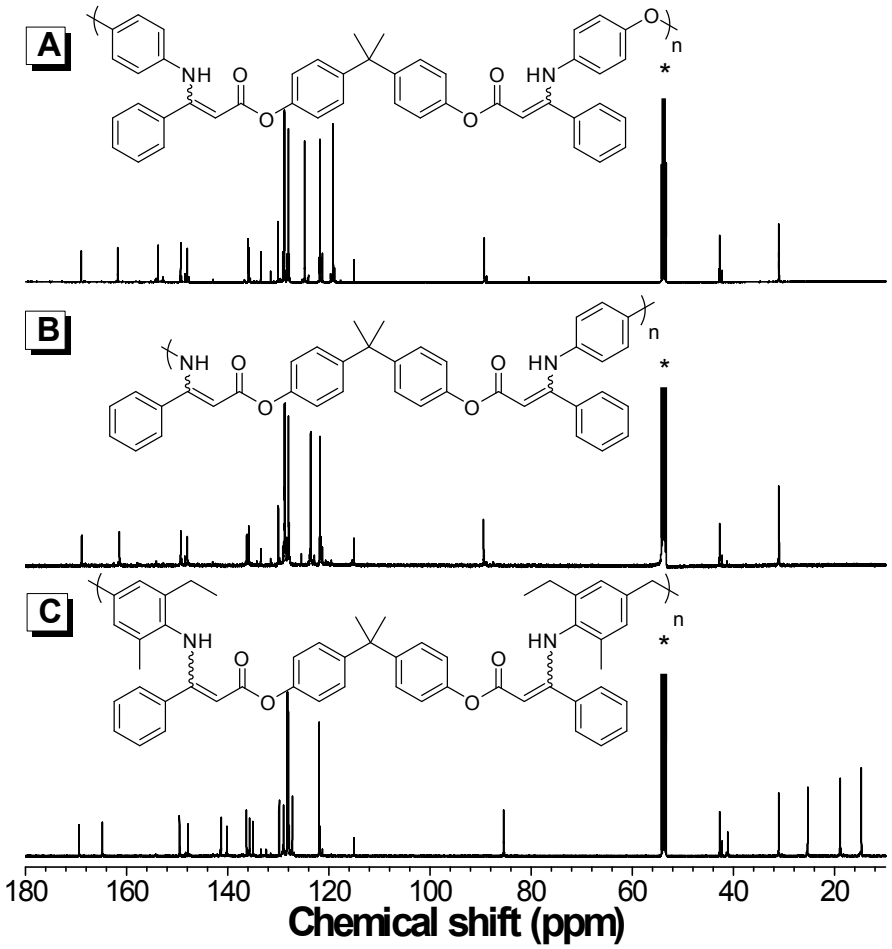

Figure S6. ^{13}C NMR spectra of (A) P**Ib**, (B) P**Ic** and (C) P**Id** in dichloromethane-d_2. The solvent peaks are marked with asterisks.