Electronic Supporting Information

Palladium-catalyzed alkyne polyannulation of diphenols and unactivated internal diynes: a new synthetic route to functional hetrocyclic polymers

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Table contents

Table S1 Crystal data and structure refinement for model compound **3**.

Empirical formula	$C_{21}H_{16}O_3S$	
Formula weight	348.40	
Temperature	173.15 K	
Wavelength	1.5418 Å	
Crystal system	Triclinic	
Space group	P–1	
Unit cell dimensions	a = 9.8165(6) Å	α= 100.954(7)°.
	b = 12.2268(10) Å	β= 94.518(6)°.
	c = 14.5725(12) Å	γ = 94.518(6)°.
Volume	1655.1(2) $Å^3$	
Z	4	
Density (calculated)	1.398 Mg/m^3	
Absorption coefficient	1.880 mm^{-1}	
F(000)	728	
Crystal size	0.30 × 0.08 × 0.04 mm^3	
Theta range for data collection	9.40 to 67.49°.	
Index ranges	-8<=h<=11, -14<=k<=14, -17<=l<=17	
Reflections collected	9565	
Independent reflections	5695 [R(int) = 0.0495]	
Completeness to theta = 66.50°	95.83 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.81802	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5695 / 0 / 453	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.1251	
R indices (all data)	R1 = 0.0823, wR2 = 0.1392	
Largest diff. peak and hole	0.625 and -0.412 e.$Å^{-3}$	

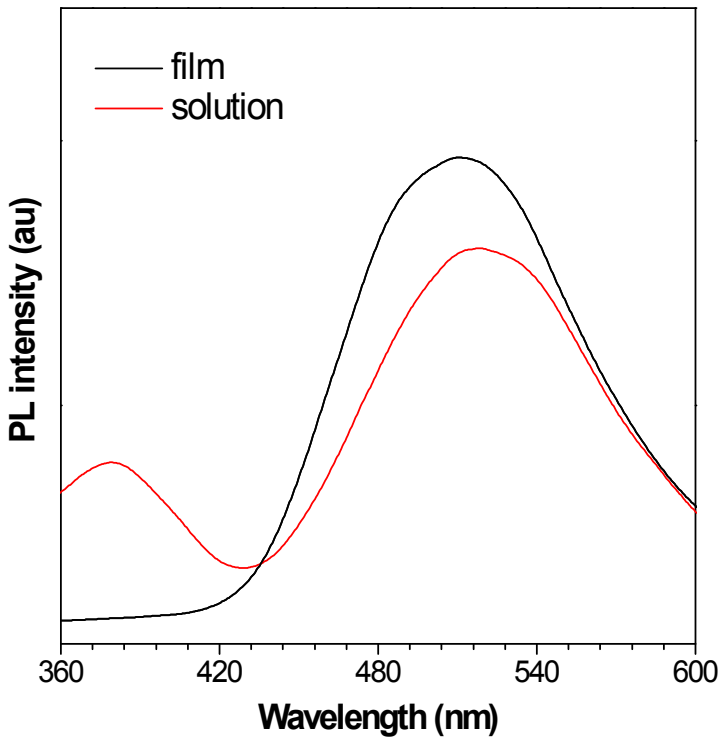

Fig. S1 Emission spectra of P**1**/**2d** in THF solution and as solid film. Solution concentration: 10 μM; excitation wavelength: 325 nm.