

Electronic Supplementary Information Organogels from unsymmetrical π -conjugated 1,3,4-oxadiazole derivatives

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Table S1. Gelation properties of 4-POXD-Bn (n= 8, 12) in different solvents.^a

	Solvents	4-POXD-B8	4-POXD-B12
Aromatic	Benzene	S	S
	Toluene	S	S
	Chlorobenzene	S	S
	Nitrobenzene	S	S
Chlorinated	Chloroform	S	S
	Dichloromethane	S	S
	1,2-dichloroethane	S	S
Alkanes	Cyclohexane	S	S
	n-heptane	P	P
esters	Ethyl acetate	S	S
	Methyl acetate	S	S
ethers	Tetrahydrofuran	S	S
	Diethyl ether	S	S
ketones	Acetone	P	P
	2- butanone	S	S
Alcohols	Glycol	I	I

^a P = precipitation; S = solution.

Table S2. Different solvent parameters.

Class of solvent	Solvents	δ_a (cal cm ⁻³) ^{1/2}	$E_T(30)^{[1]}$ (kcal mol ⁻¹)	ϵ
Aromatic	Benzene	1	34.5	2.27
	Toluene	1.22	33.9	2.379
	Chlorobenzene	2.33	38.1	5.6
	Nitrobenzene	4.65	42	34.8
Chlorinated	Chloroform	3.18	39.1	4.806
	Dichloromethane	4.31	38.1	9.08
	1,2-dichloroethane	4.12	41.3	10.37
Alkanes	Cyclohexane	0.1	31.2	2.1
esters	Ethyl acetate	4.36	38.1	---
	Methyl acetate	4.36	40.0	---
ethers	Tetrahydrofuran	4.8	37.4	
	Diethyl ether	2.87	34.6	4.335

ketones	Acetone	6.13	42.2	---
alcohols	Glycol	13.8	56.3	41.4
	Methanol	12.44	55.4	33.62
	Ethanol	10.43	51.6	25.07
	n-propanol	9.12	50.7	20.8
	n-butanol	8.19	50.2	17.84
Others	Acetonitrile	9.3	45.6	38.8
	Dimethylformamide	8,67	43.8	37.6
	Dimethylsulfoxide	9.43	45.1	48.9

Table S3. Gibbs energies of solvation of hexane in various solvents at 298K in kJ/mol

Class of solvent	Solvents	Gibbs energies (ΔG_{solv})
Aromatic	Benzene	-1.2
	Toluene	-2.6
	Chlorobenzene	-2.0
	Nitrobenzene	0.4
Chlorinated	Chloroform	-2.2
	Dichloromethane	---
	1,2-dichloroethane	0.1
Alkanes	Cyclohexane	-3.5
esters	Ethyl acetate	-0.8
	Methyl acetate	---
ethers	Tetrahydrofuran	-2.1
	Diethyl ether	---
ketones	Acetone	0.9
alcohols	Glycol	11.9
	Methanol	4.2
	Ethanol	2.2
	n-propanol	1.4
	n-butanol	0.0
Others	Acetonitrile	4.1
	Dimethylformamide	3.2
	Dimethylsulfoxide	7.3



Fig. S1. Gel images of 4-POXD-B8 in various solvents.

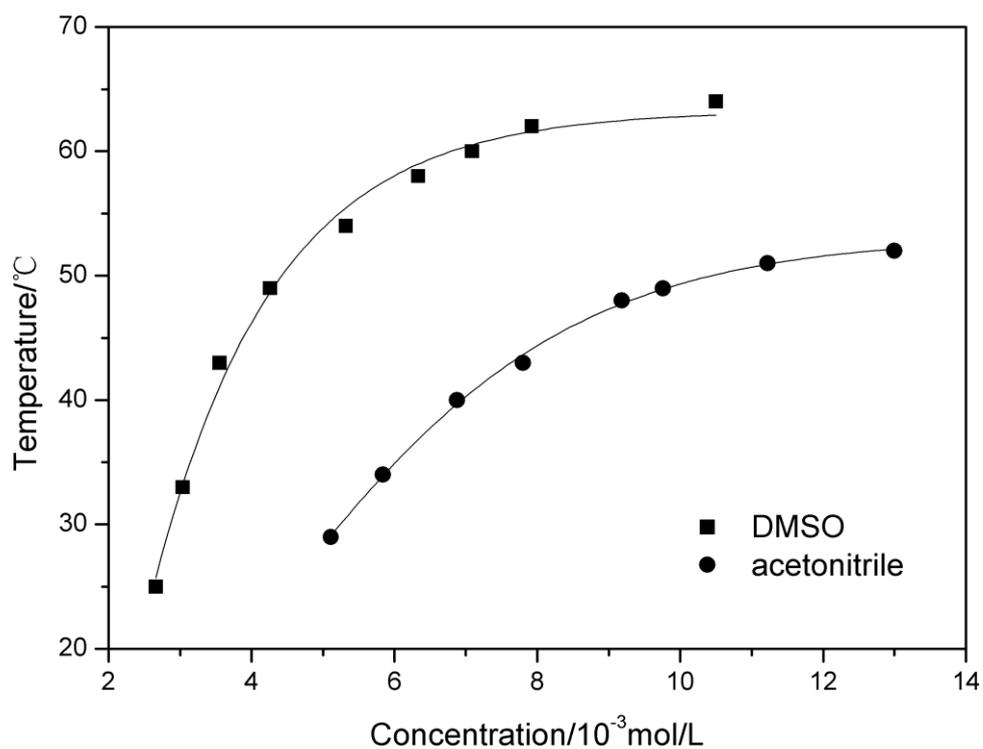


Fig. S2. Gel-sol phase-transition curves of 4-POXD-B12 in DMSO, acetonitrile.

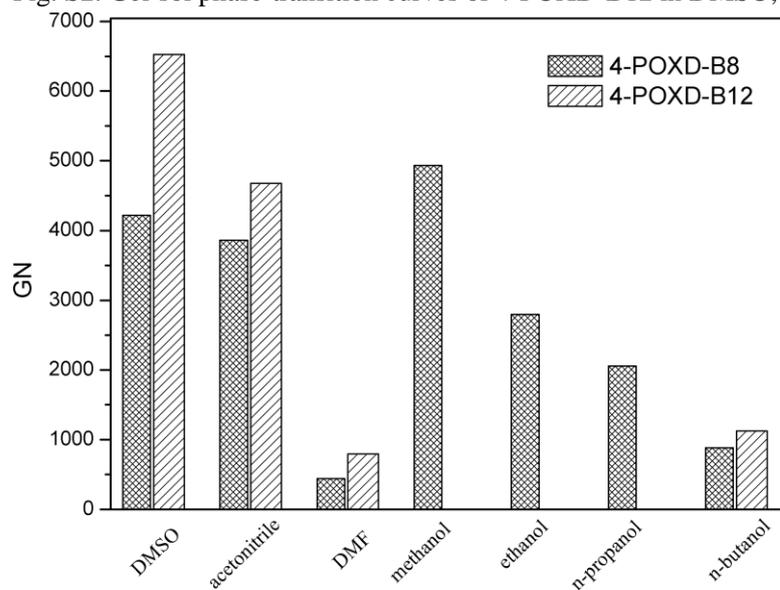


Fig. S3. GN for gelators 4-POXD-Bn (n = 8, 12) in the studied solvents.

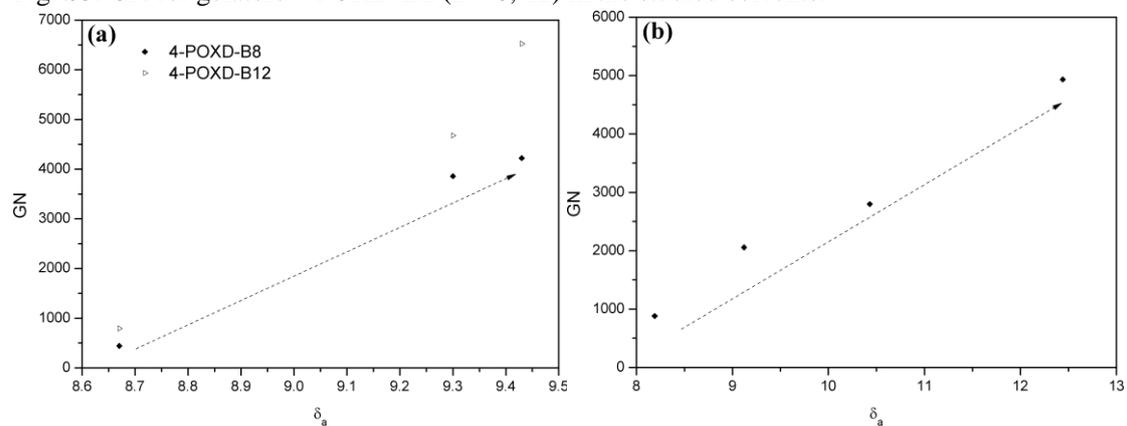


Fig. S4. Effect of the polar solubility parameter δ_a on GN of gelator 4-POXD-Bn. (a) “other” solvents, (b) alcohol solvents.

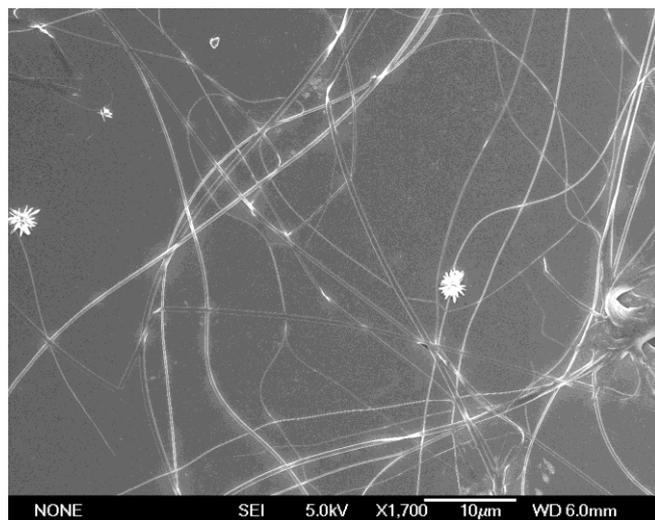


Fig. S5. SEM images of 4-POXD-B8 on Si underlay after solvent had evaporated from 1.8×10^{-4} mol/L DMSO solutions of the compound drop cast on the surface. (Solvent evaporated at room-temperature)

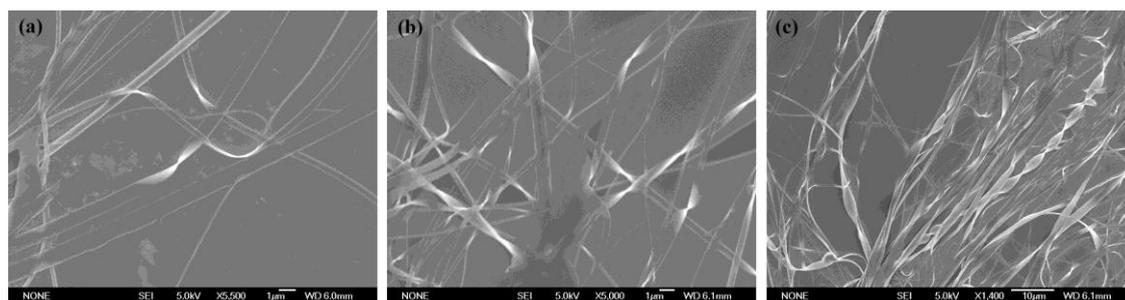


Fig S6. SEM images of 4-POXD-B8 on Si underlay after solvent had evaporated from (a) 1.8×10^{-4} mol/L, (b) 5.3×10^{-4} mol/L, and (c) 1.0×10^{-3} mol/L DMSO solutions of the compound drop cast on the surface. (Solvent evaporated at room-temperature)

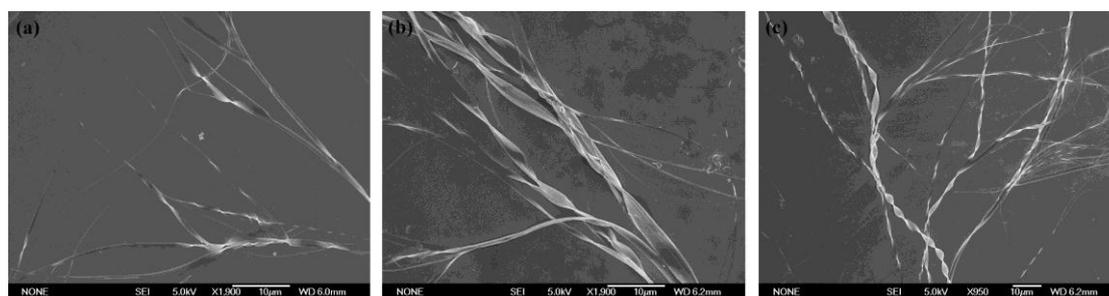


Fig. S7. SEM images of 4-POXD-B8 on Si underlay after solvent had evaporated from (a), (b) 1.1×10^{-4} mol/L and (c) 2.3×10^{-4} mol/L DMF solutions of the compound drop cast on the surface. (Solvent evaporated at room-temperature)

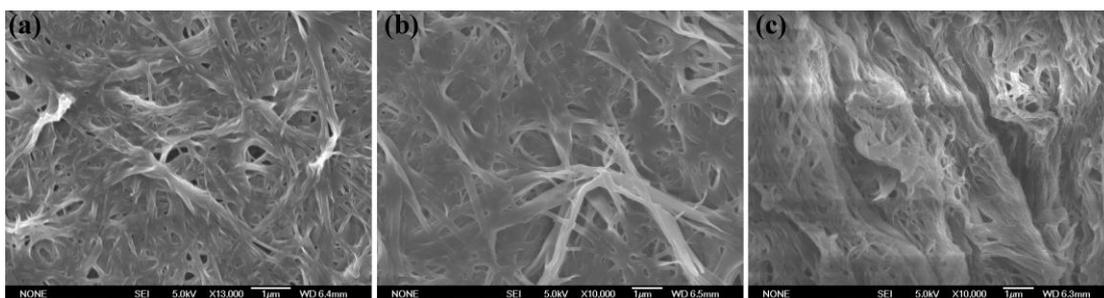


Fig. S8. SEM images of 4-POXD-B12 xerogels from (a) DMSO, (b) acetonitrile, and (c) DMF.

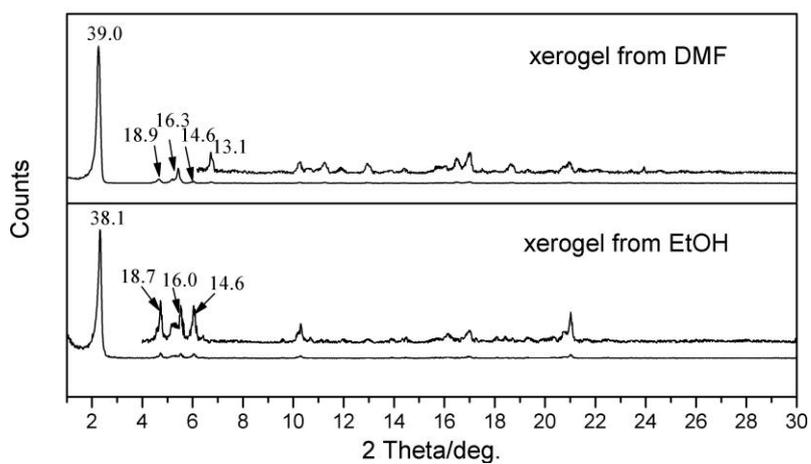


Fig. S9. X-Ray diffraction (XRD) spectra of 4-POXD-B8 xerogels from DMF and ethanol.

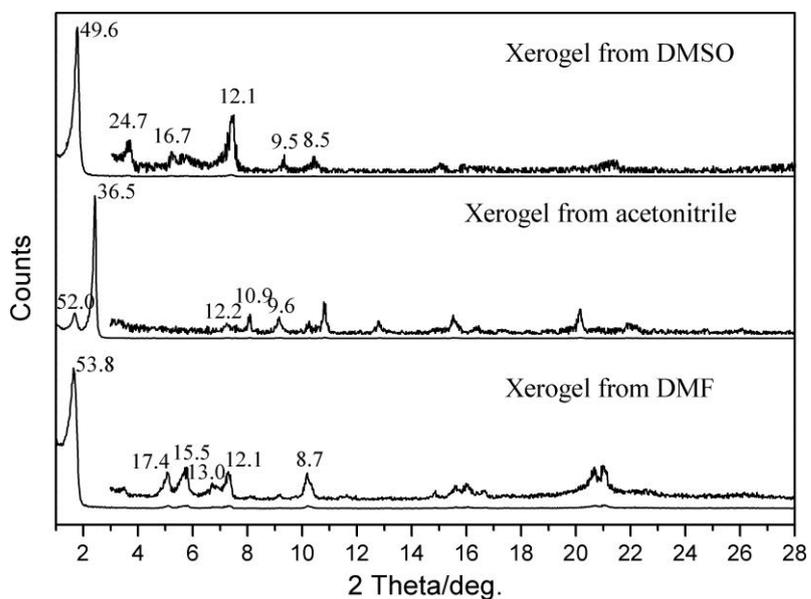


Fig. S10. X-Ray diffraction (XRD) spectra of 4-POXD-B12 xerogels from DMSO, acetonitrile and DMF.

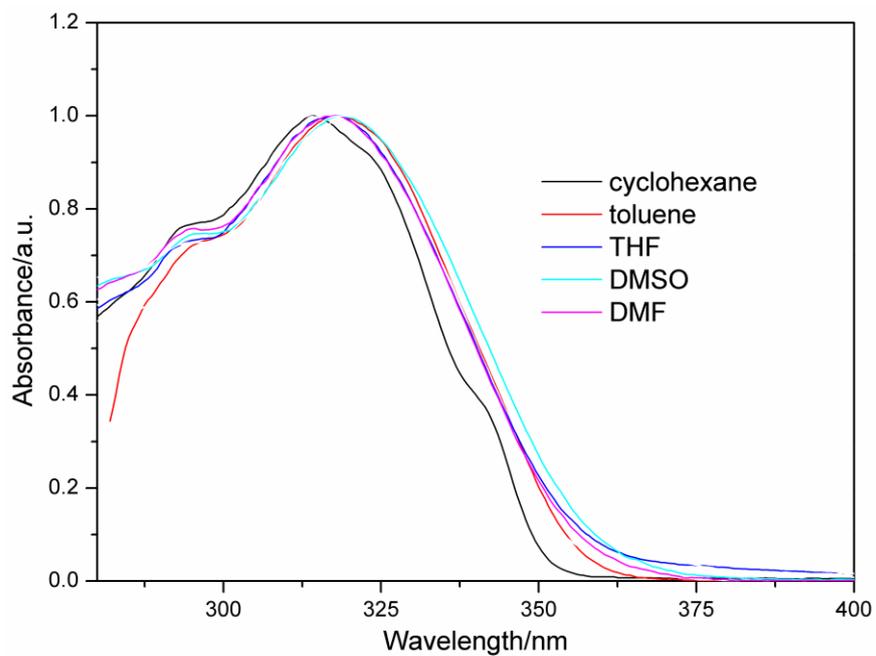


Fig. S11. UV-vis spectra of 4-POXD-B8 in aprotic solvents.

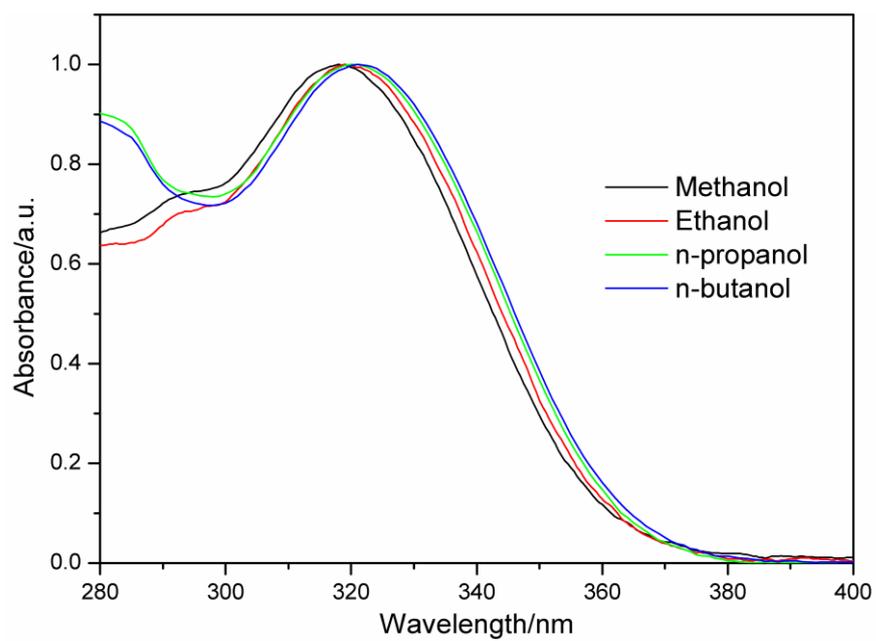


Fig. S12. UV-vis spectra of 4-POXD-B8 in protic solvents.

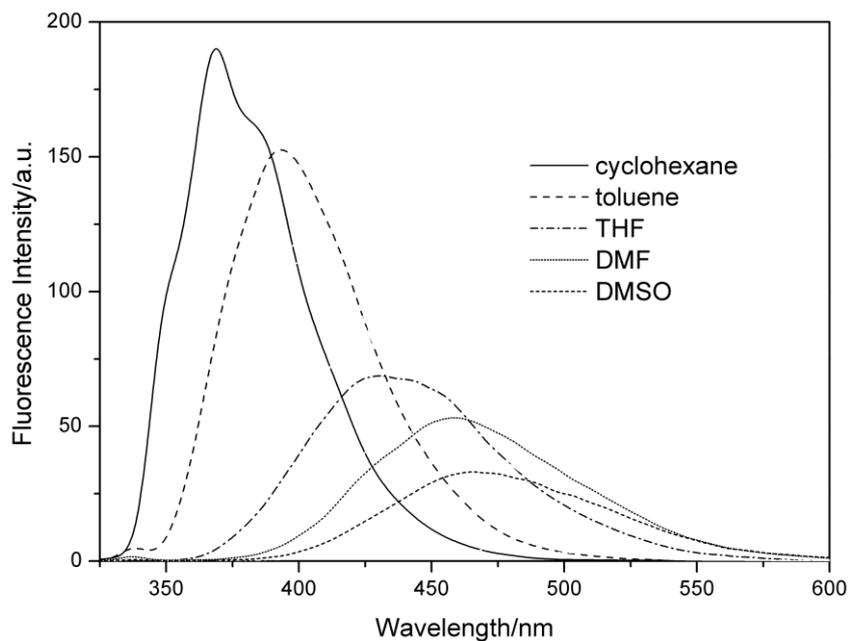


Fig. S13. FL spectra of 4-POXD-B8 in different solvents at a concentration of 1×10^{-5} mol/L at room temperature.

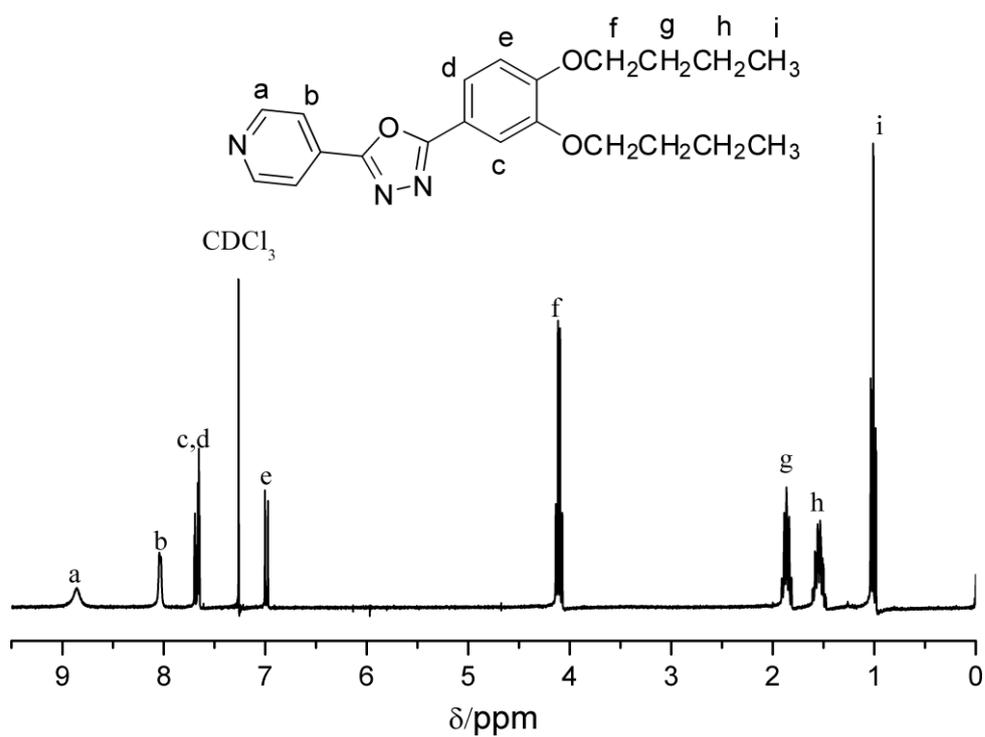


Fig. S14. ^1H NMR spectrum of 4-POXD-B4 in CDCl_3 .

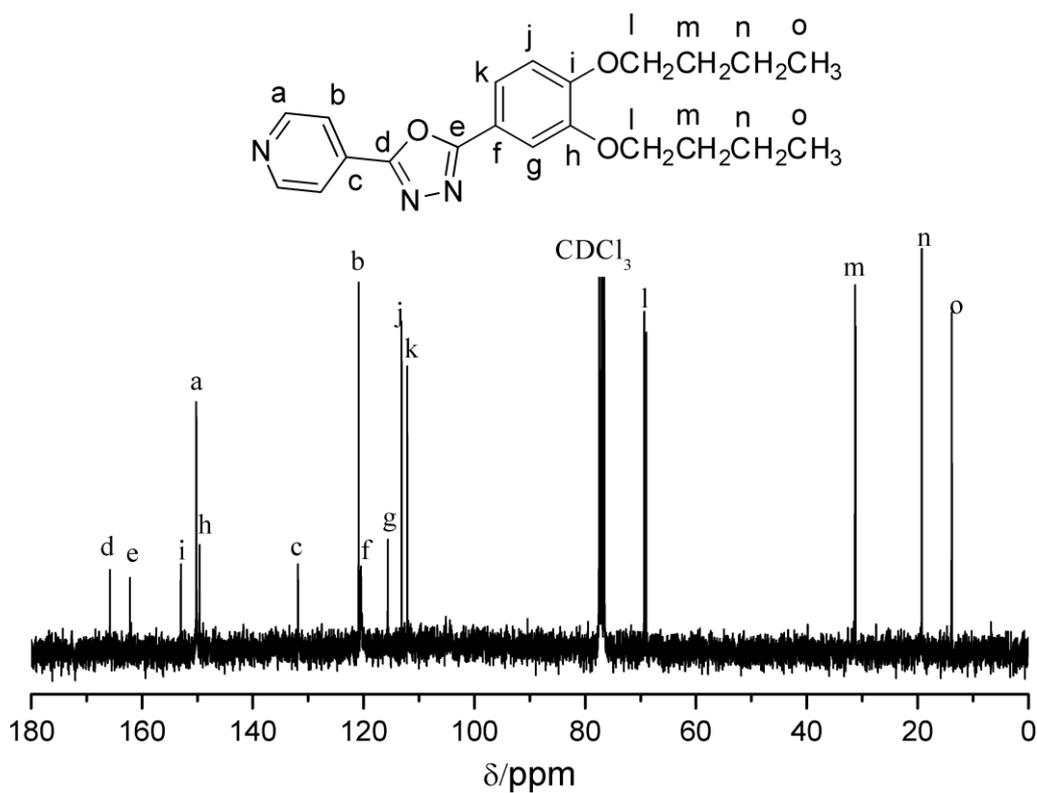


Fig. S15. ^{13}C NMR spectrum of 4-POXD-B4 in CDCl_3 .

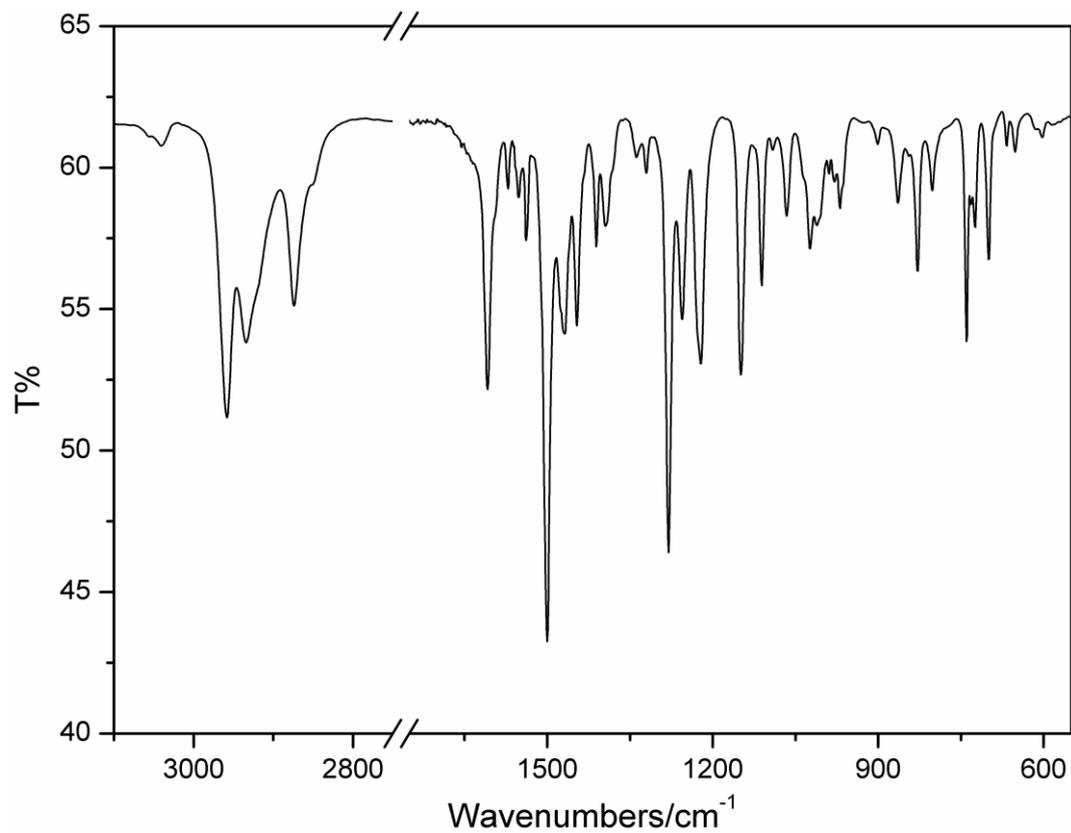


Fig. S16. FTIR spectrum of 4-POXD-B4 powder.

[1] Reichardt, C. solvents and solvent effects in organic chemistry, 3rd ed, Wiley-VCH: New York, 2003.