

Supporting Information

Selenium-containing Polyimides with an Ultrahigh Intrinsic Refractive Index

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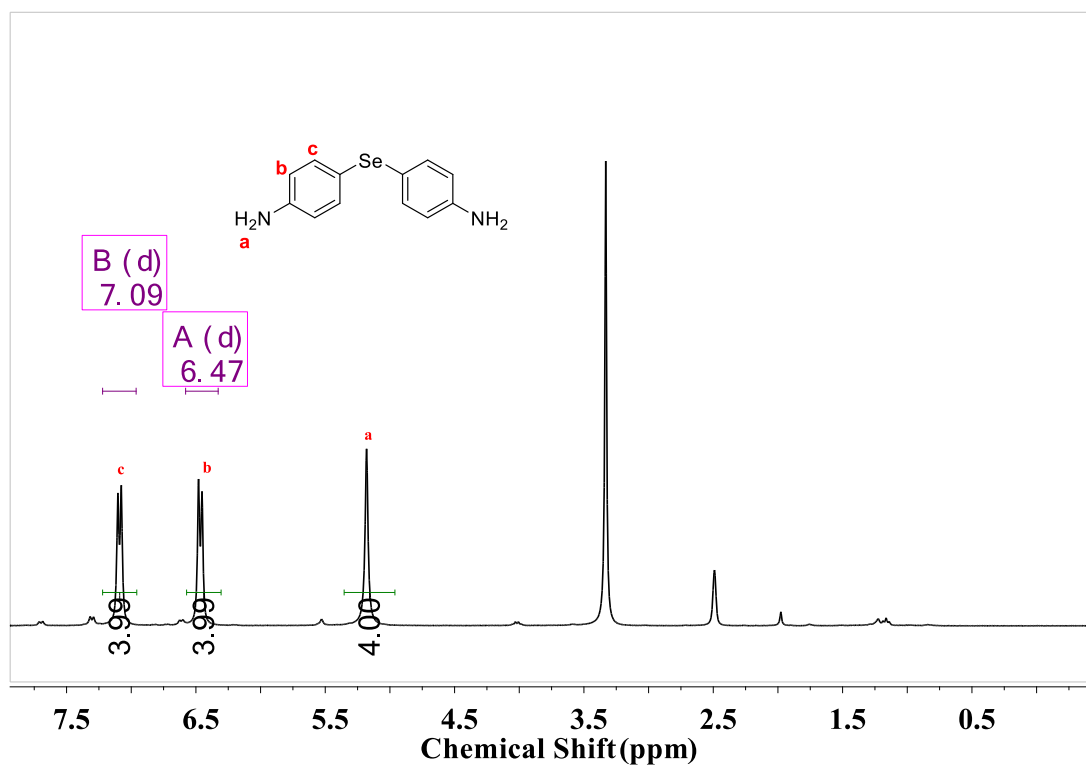


Figure S1. ^1H NMR of BAPSe in DMSO-d_6 .

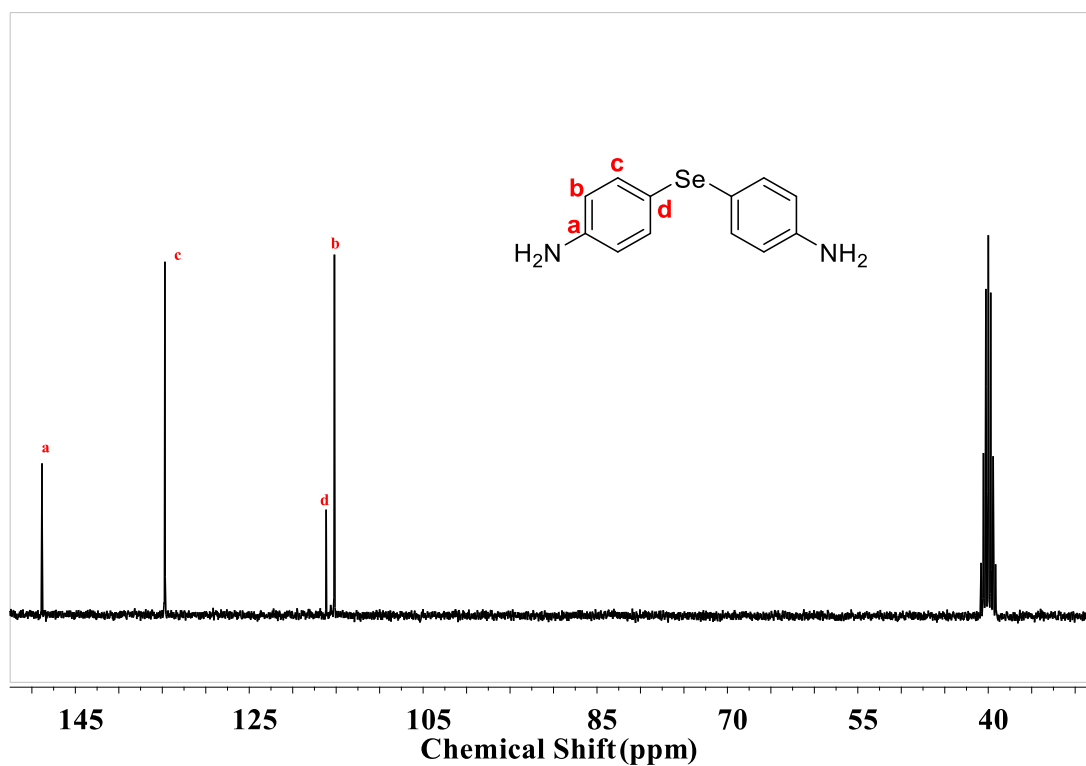


Figure S2. ^{13}C NMR of BAPSe in DMSO-d_6 .

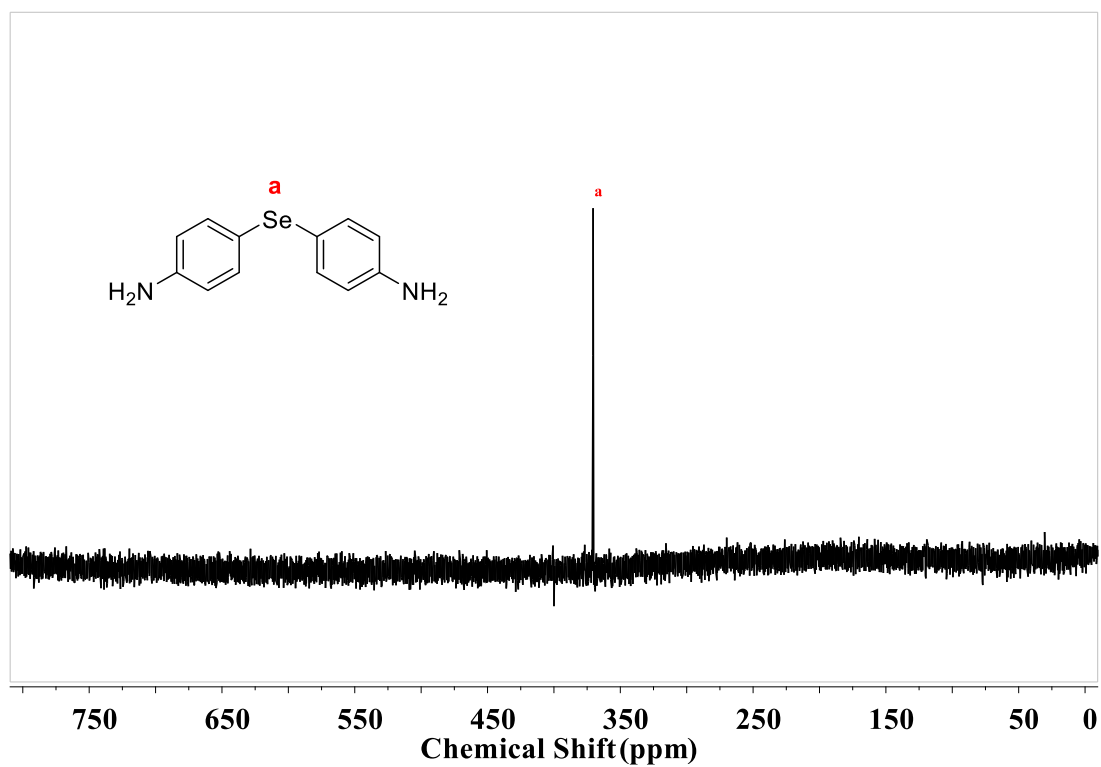


Figure S3. ^{77}Se NMR of BAPSe in DMSO-d_6 .

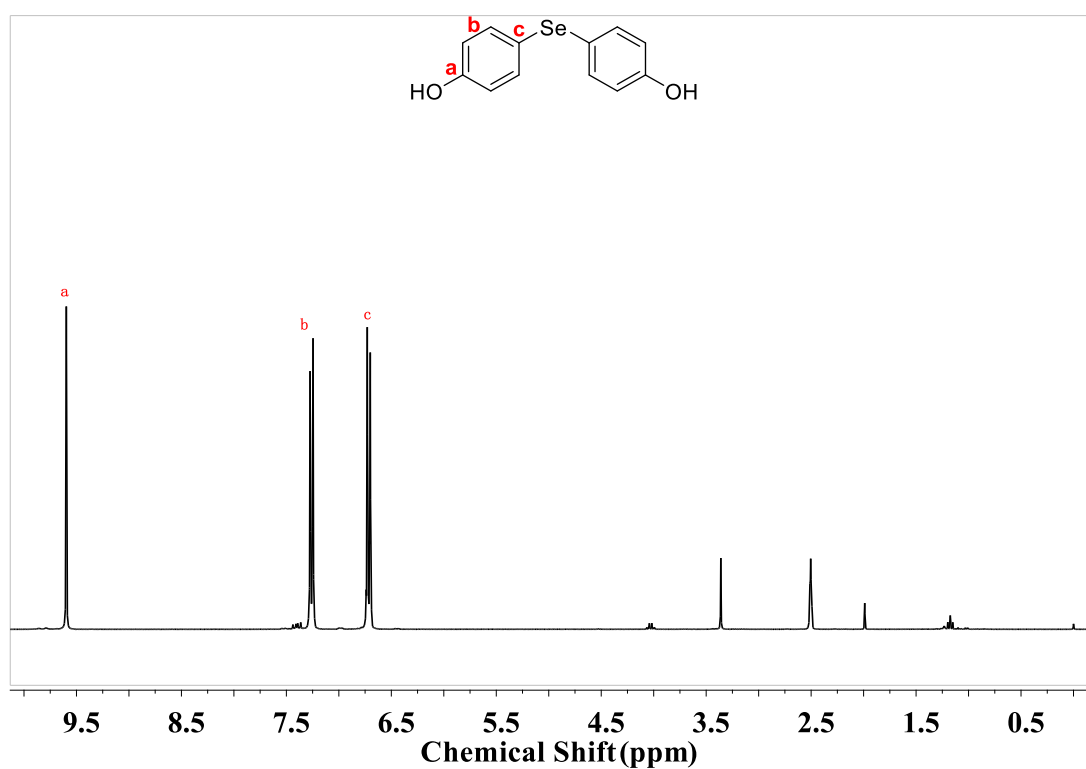


Figure S4. ^1H NMR of BHPSe in DMSO-d_6 .

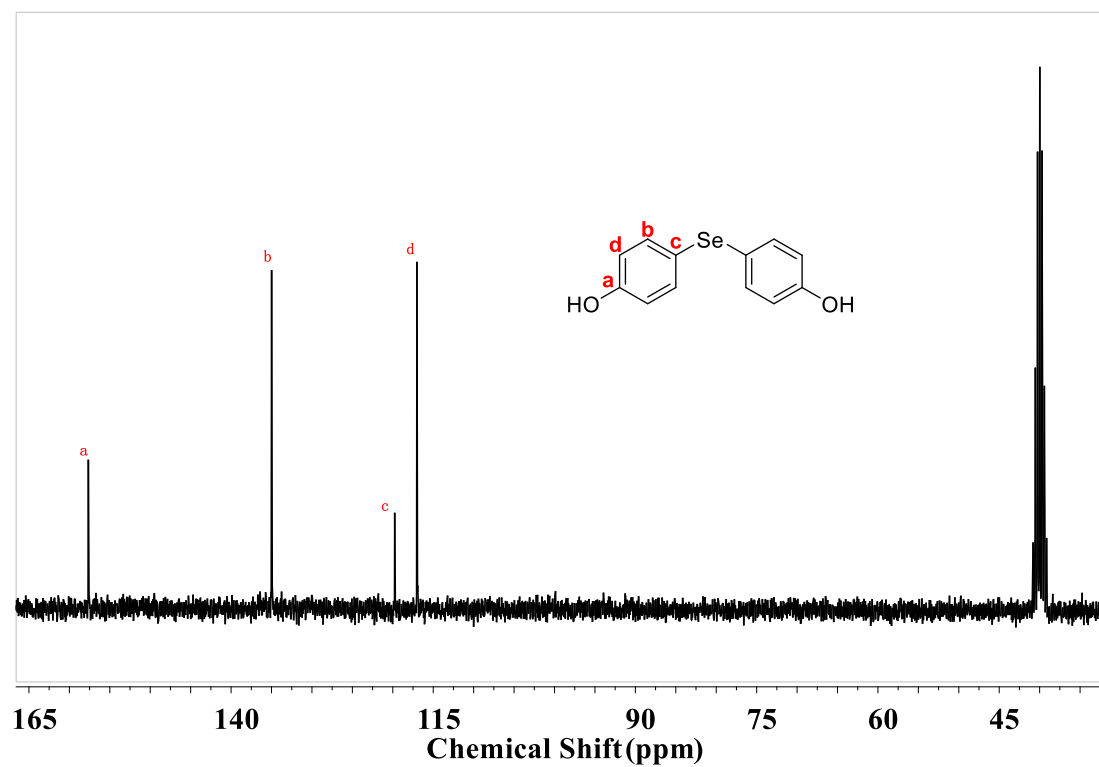


Figure S5. ^{13}C NMR of BHPSe in DMSO-d_6 .

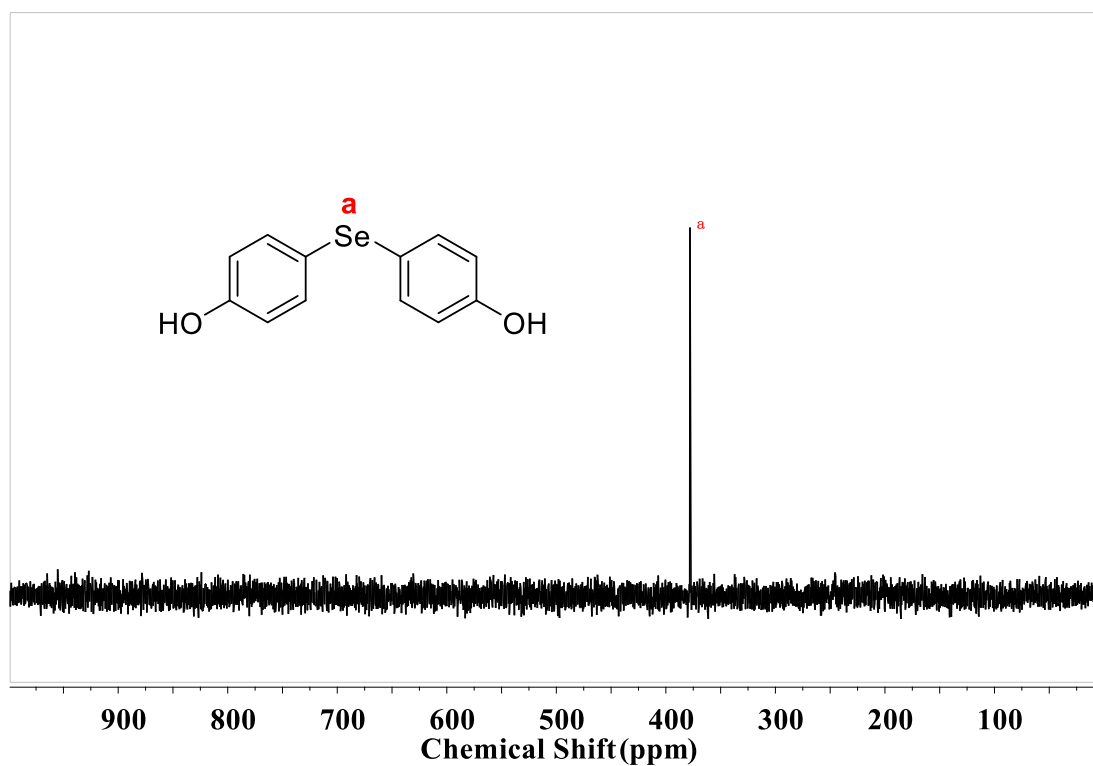


Figure S6. ^{77}Se NMR of BHPSe in DMSO-d_6 .

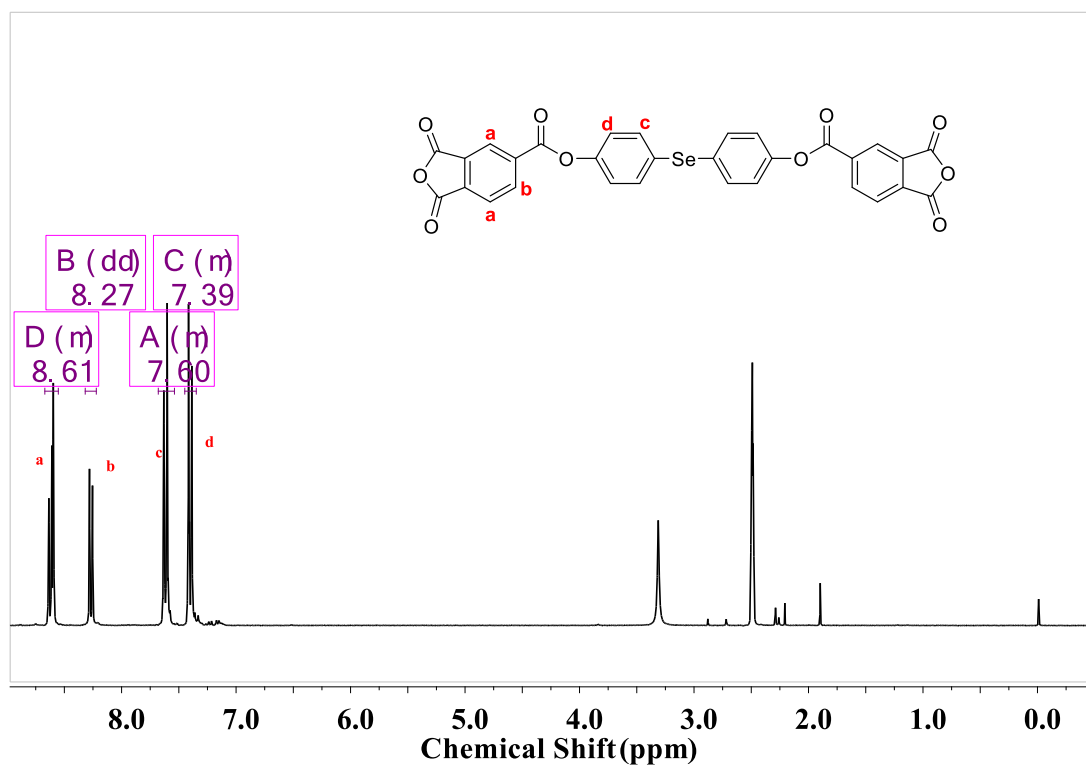


Figure S7. ^1H NMR of BDPSD in DMSO-d_6 .

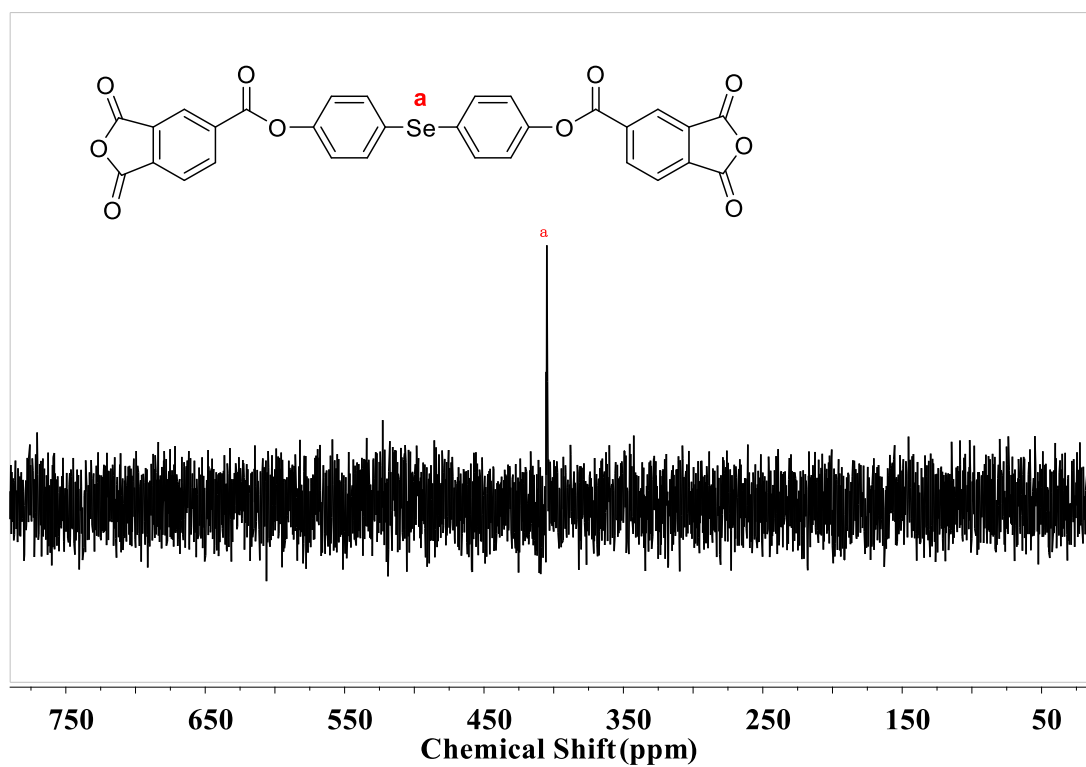
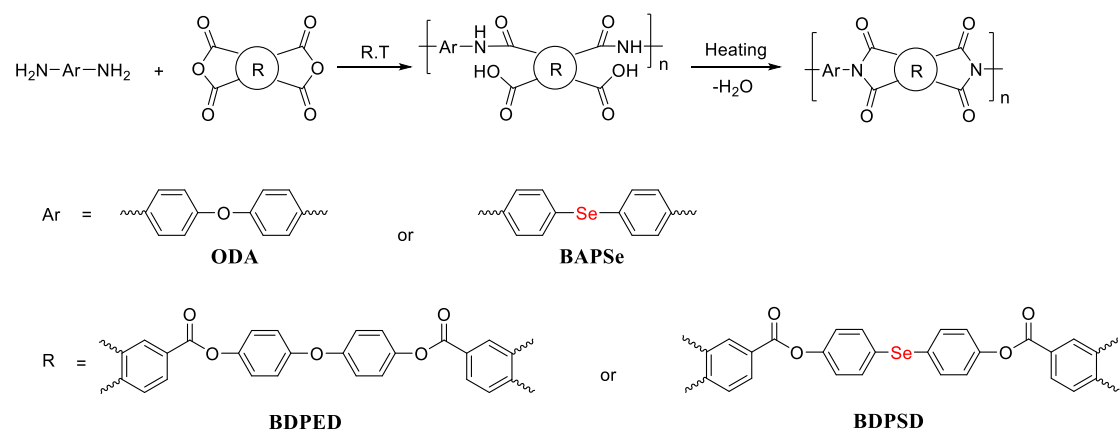
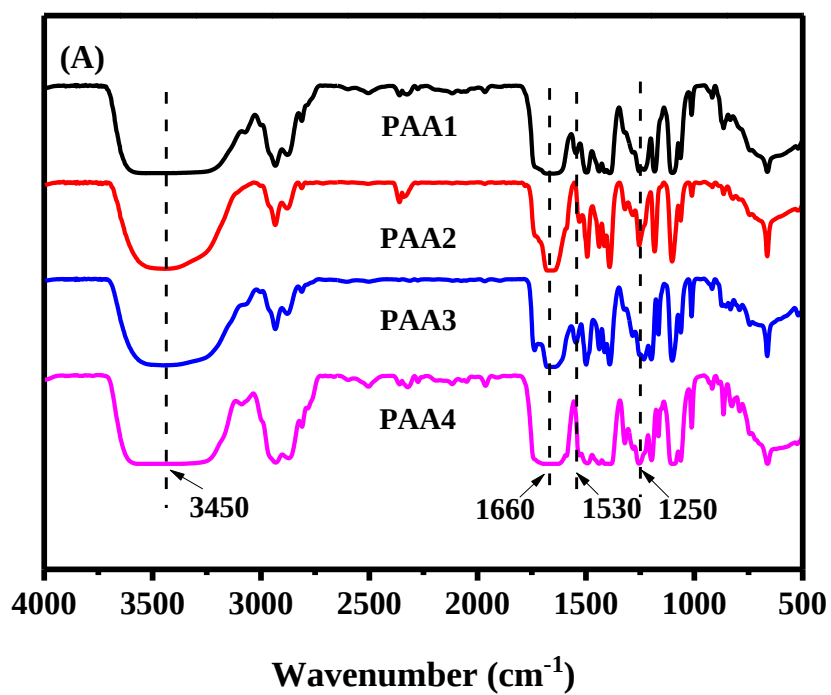


Figure S8. ^{77}Se NMR of BDPSD in DMSO-d_6 .



Scheme S2. Preparation procedures and the structures of four PIs with different contents and location of selenium in their repeat units.



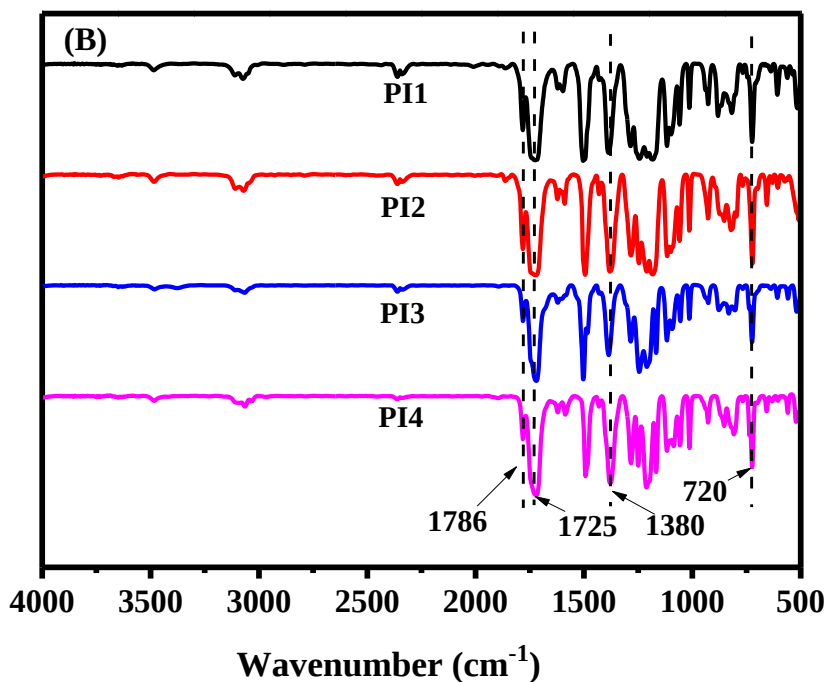


Figure S10. FT-IR spectra of four synthesized PAAs (PAA1-4) (A) and four synthesized PIs (PI1-4) (B) films on the potassium bromide tablet.

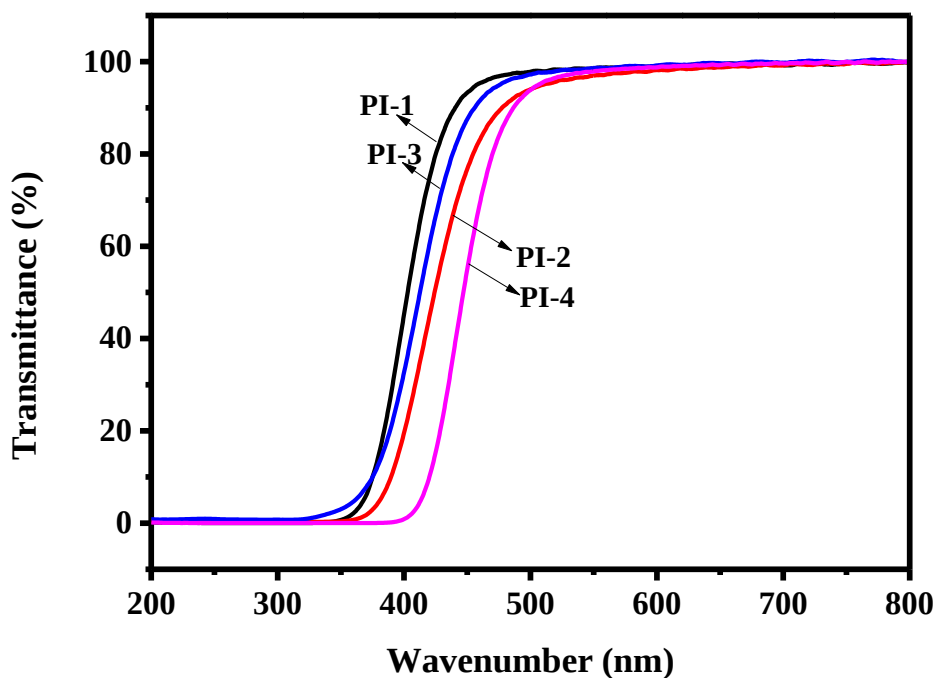


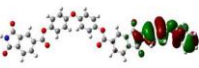
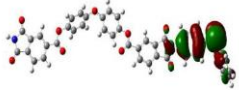
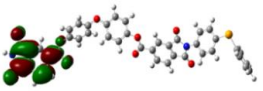
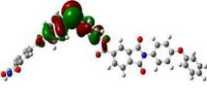
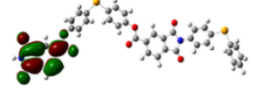
Figure S11. UV-vis spectra of four synthesized PIs with about 2 μm thickness.

Table S1. Optical Transmittance, Absorption Edges (λ_E), Calculated Molecular Orbital Energies (ϵ) of HOMO and LUMO and Energy Band Gaps ($\Delta\epsilon$) for Monomeric Models of four synthesized PIs.

PIs	T ₄₀₀ (%) ^a	T ₂₀₀ (%) ^b	λ_E^c (nm)	ϵ_{HOMO} (eV)	ϵ_{LUMO} (eV)	$\Delta\epsilon$ (eV)
PI-1	45.2	0.2	434	-6.30	-3.11	3.19
PI-2	19.5	0.4	466	-5.91	-3.12	2.79
PI-3	32.6	0.8	451	-6.09	-3.15	2.94
PI-4	0.9	0.1	477	-5.92	-3.15	2.77

^a Transmittance at 400 nm; ^b Transmittance at 200 nm; ^c the intersection of tangent line of the absorption curve and initial curve.

Table S2. Molecular orbital (MO) diagrams of four synthesized PIs.

PIs	HOMO	LUMO	Length (Å) ^a	Dihedral angle (°) ^b	
				Dianhydride	Diamine
PI-1			33.19	52.68	66.94
PI-2			32.43	57.06	66.46
PI-3			31.26	40.59	60.19
PI-4			30.46	51.19	81.75

^a The linear length of one repeat unit in HOMO state.

^b Dihedral angle between adjacent phenyl group in HOMO of repeat unit.

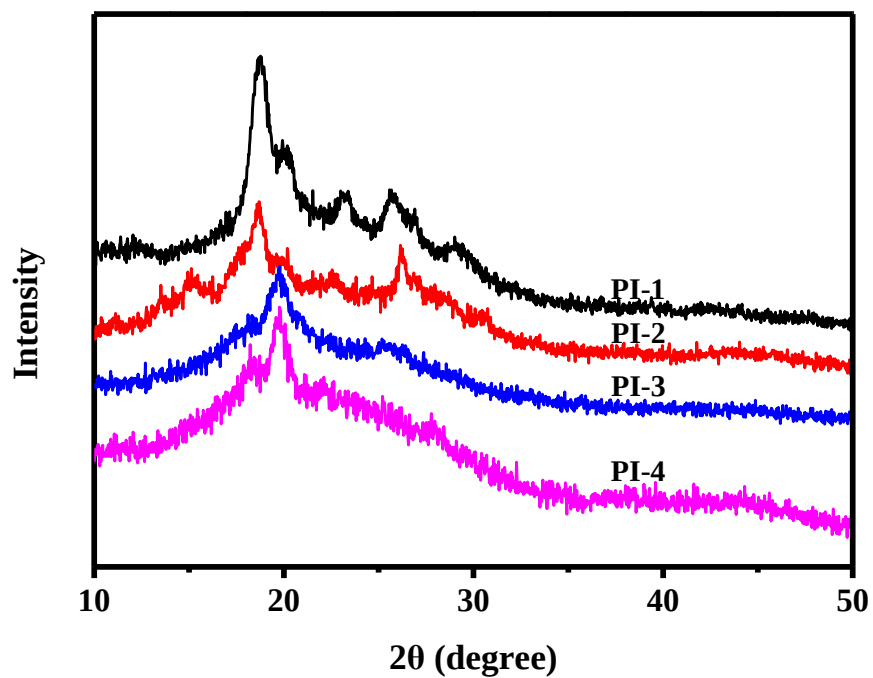


Figure S12. WAXD profiles of four synthesized PIs.

Table S3. Solubility of four synthesized PIs^a.

PIs	DMSO	DMAc	DMF	NMPc	m-Cresol	THF	CHCl ₃	Acetone
1	-	-	-	-	-	-	-	-
2	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-
4	-	-	-	-	-	-	-	-

^a Qualitative solubility measured with 10 mg of the PIs in 1mL of solvent. -, insoluble at room temperature and heating.

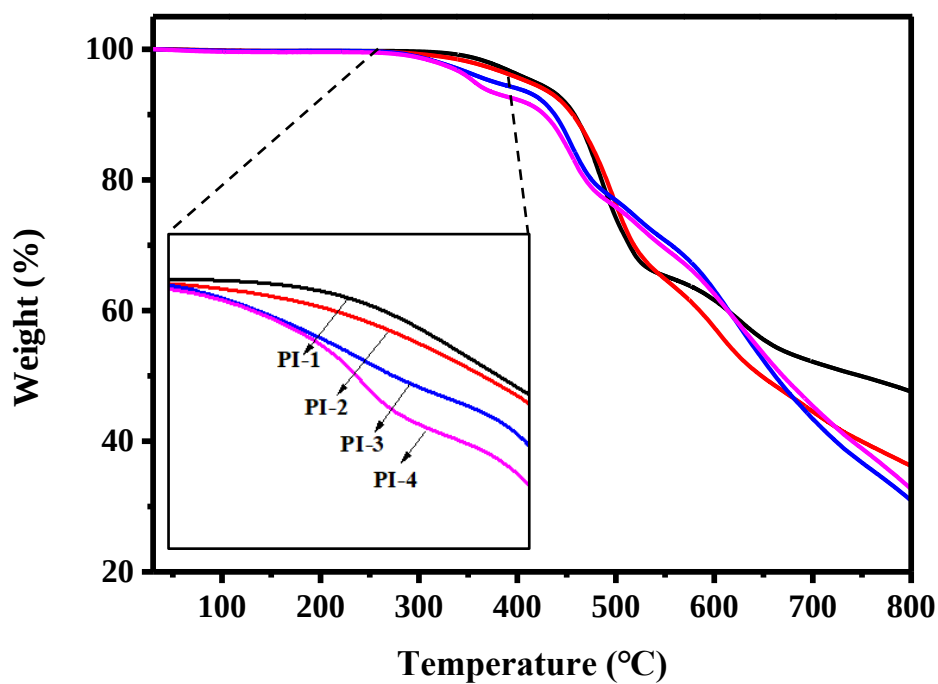


Figure S13. TGA thermographs of four synthesized PIs with N₂ atmosphere.

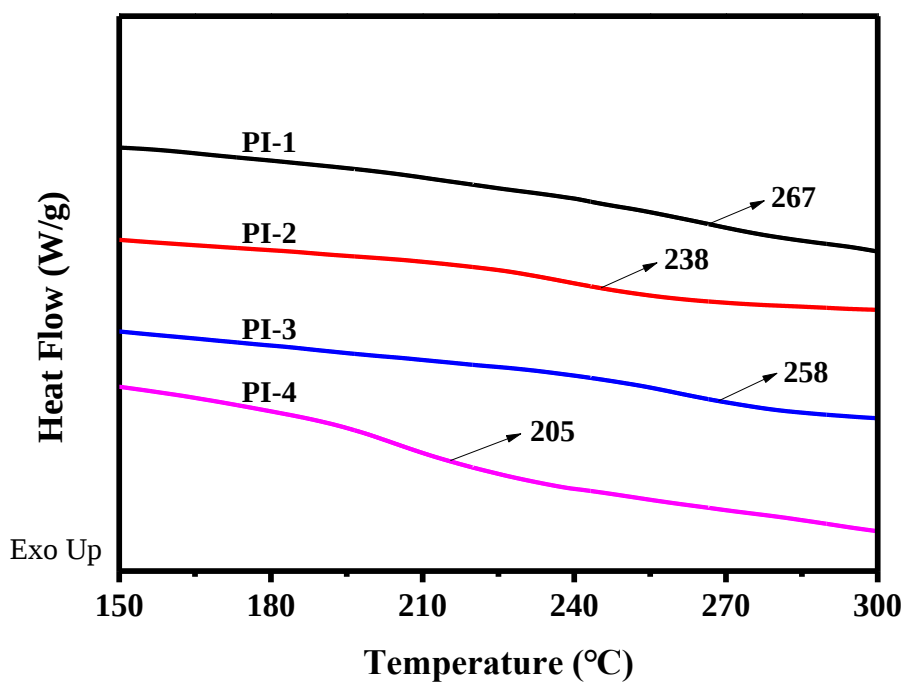


Figure S14. DSC thermographs of four synthesized PIs with N₂ atmosphere. Glass transition temperature of four PIs were labeled.

Table S4. Thermal properties of four synthesized PIs^a

PIs	T_g (°C)	T_d^5(°C)	T_d^{10}(°C)	Char yield (%)
PI-1	267	417	457	47.5
PI-2	238	411	456	36.2
PI-3	258	376	438	30.8
PI-4	205	356	438	32.5

^a T_g , glass transition temperature of four PIs; T_d^5 , the temperature at 5% weight loss; T_d^{10} , the temperature at 10% weight loss; Char yield, residual weight percentage at 800 °C in N₂ atmosphere.