

Electronic Supplementary Information

Dual Aggregation-Induced Emission Enhancement (AIEE) and Crosslink-Enhanced Emission (CEE) Driven via Halogen-Bond-Assisted Cocrystallization and Radical Solid-Phase Polymerization

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1. Materials

trans-4,4'-Dibromostilbene (DBSB) (95%, Sigma-Aldrich, USA), 2,5-dibromoterephthalaldehyde (DBTPA) (>97%, Tokyo Chemical Industry (TCI), Japan), *trans*-4-bromocinnamaldehyde (BCA) (97%, Sigma-Aldrich), 5-bromo-2,3-dimethoxybenzaldehyde (BDMB) (97%, Sigma-Aldrich), 1,2,4,5-tetrabromobenzene (4BB) (97%, Sigma-Aldrich), 1,4-diiodotetrafluorobenzene (I-C₆F₄-I) (98%, Sigma-Aldrich), 4-vinylpyridine (4VP) (95%, Sigma-Aldrich), 1-vinyl-2-pyrrolidone (NVP) (>99%, TCI), 2,2-dimethoxy-2-phenylacetophenone (DMPA) (99%, Sigma-Aldrich), ethylene glycol dimethacrylate (EGDMA) (98%, Sigma-Aldrich), dichloromethane (CH₂Cl₂) (99.8%, Fisher Scientific, USA), ethanol (≥99.5%, absolute, Fisher Scientific), *N,N*-dimethylformamide (DMF) (>99.5%, Kanto Chemical, Japan), toluene (HPLC grade, ≥99.5%, Fisher Scientific), ethanol (EtOH) (≥99.5%, absolute, Fisher Scientific), hexane (>99%, International Scientific, Singapore) α,α,α -trifluorotoluene (or trifluoromethylbenzene) (PhCF₃) (≥99%, Sigma-Aldrich), deuterated chloroform (CDCl₃) (99.8%D, Cambridge Isotope Laboratories, USA), deuterated dimethyl sulfoxide (DMSO-*d*₆) (99.9%D, Cambridge Isotope Laboratories), lithium bromide (LiBr) (>99%, TCI), potassium bromide (KBr) (≥99%, trace metals basis, Sigma-Aldrich), poly(4-vinyl pyridine) (P4VP) (molecular weight = ca. 60000) (Sigma-Aldrich), and poly(methyl methacrylate) (PMMA) (molecular weight = ca. 50000, nominal M_p = 46890) (Agilent, US) were used as received.

2. Measurement

¹H NMR spectra were recorded at room temperature on a Bruker (Germany) BBFO400 spectrometer (400 MHz) and AV400 spectrometer (400 MHz). CDCl₃ and DMSO-*d*₆ were used as NMR solvents. The residual non-deuterated solvents were used as the internal standards for ¹H NMR analysis.

The GPC analysis was performed on a Shimadzu (Kyoto, Japan) LC-2030C Plus liquid chromatograph equipped with two Shodex LF-804 columns (300 × 8.0 mm; bead size = 6 μm; pore size = 1500 Å) and one Shodex KD-802 column (300 × 8.0 mm; bead size = 6 μm; pore size = 150 Å) (DMF). The eluent was DMF (containing 10 mM of LiBr) at a flow rate of 0.34 mL/min (40 °C). Sample detection was conducted using a Shimadzu differential refractometer detector RID-20A. The column system was calibrated with standard polystyrenes.

The Fourier-transform infrared spectroscopy (FTIR) was carried out on a Bruker (Bruker, US) ALPHA FTIR spectrometer. KBr was used as a matrix for FTIR.

The UV light source was a UV-LED light (365 (± 10) nm wavelength, 900 mW/cm², C14052-0-A5 models (Hamamatsu Photonics, Japan)). The polymer sheets were moulded using a 2T Mini-Pellet Press (Specac, UK) with a diameter of 7 mm.

The thermal analysis of the polymers were performed with a thermal gravimetric analysis (TGA) Q500 (TA instrument, New Castle, US). The TGA analysis was carried out in platinum pans under flowing air from 25 to 600 °C.

The fluorescence spectra in solid state were measured using a Fluoromax 4 spectrometer (HORIBA, Japan). The excitation wavelengths were 405 nm and 488 nm. The sample masses were 0.10 g. All the samples were rounded shape (diameter 7 mm and thickness 1 mm).

Confocal Raman spectroscopy: Raman spectra were recorded in the 100–3000 cm⁻¹ range using a LabRAM HR Evolution Raman microscope equipped with an Olympus BX41 optical microscope and a 100× objective. A 633 nm helium–neon laser was used as excitation source for all experiments.

The confocal fluorescence images were taken with Zeiss LSM 710 Confocal (Observer Z1, Germany) using the filter set 38 under autoexposure. The laser filters used are a green laser filter (excitation wavelength (λ_{ex}) = 488 nm and emission wavelength (λ_{em}) = 493–635 nm)

and a blue laser filter ($\lambda_{\text{ex}} = 405 \text{ nm}$ and $\lambda_{\text{em}} = 410\text{--}585 \text{ nm}$). The emission intensities were analyzed using Zeiss ZEN blue software at $\lambda_{\text{em}} = 564 \text{ nm}$ and 498 nm .

The powder X-ray diffraction (PXRD) analysis was carried out with a BRUKER D8 ADVANCE (Bruker) from 10.000° to 79.994° (step size 0.020) using $\text{CuK}\alpha$ radiation ($\lambda = 1.541874 \text{ \AA}$). The parameters (2θ) and full width of half maximum (FWHM) shown in Table S2 were obtained from the PXRD spectra and data calculated from Match! software. The crystallite size was calculated using the modified Scherrer equation (least square). The distance/plane spacing between layers (d_{hkl}), microstrain (ε), crystallite size (D), and dislocation density (δ) were calculated from the following formula:

$$\text{Scherrer equation: } \ln \beta = \ln \frac{1}{\cos \theta} + \ln \frac{K\lambda}{D} = \ln \frac{1}{\cos \theta} + \text{intercept } b \quad (1)$$

$$\text{Crystallite size } (D) = \frac{K\lambda}{e^{\text{intercept } b}} \text{ [nm]} \quad (2)$$

$$\text{Layer spacing } (d_{\text{hkl}}) = \frac{n\lambda}{2\sin\theta} \text{ [nm]} \quad (3)$$

$$\text{Microstrain } (\varepsilon) = \frac{\text{radians(FWHM)}}{4\tan\theta} \quad (4)$$

$$\text{Dislocation density } (\delta) = \frac{1}{D^2} \text{ [nm}^{-2}\text{]} \quad (5)$$

Where:

β is the radians of FWHM;

θ is the incident angle (the angle between the incident ray and the scatter plane) [$^\circ$];

K is the Scherrer constant, which is a dimensionless shape factor ($K = 0.9$);

λ is the radiation wavelength ($\lambda = 0.1541874 \text{ nm}$);

D is crystallite size [nm] in the powder sample and was obtained from the intercept of the plot of $\ln\beta$ vs $\ln(1/\cos\theta)$ according to equation (1) (or (2));

n is an integer ($n = 1$).

3. Synthetic Procedures¹

General Procedure for Synthesis of Four-Component Monomer Cocrystal Solids Using Five Linkers (1–5) and Two Vinyl Monomers (6–7) via Evaporation Method

In a typical run, linker **1** (0.634 g, 1.88 mmol), monomer **7** (0.417 g, 3.75 mmol), photoinitiator DMPA (14.4 mg, 56.2 μ mol), and a crosslinkable monomer EGDMA (0.297 g, 1.50 mmol) were dissolved in dichloromethane (18.75 mL) in a flask. Slow evaporation of dichloromethane was performed using a rotary evaporator to obtain a four-component monomer solid (**1·7·DMPA·EGDMA**) within one hour. The four-component solids of other monomer cocrystal solids were prepared similarly (with the Br/monomer molar ratio = 1/1).

General Procedure for Free-Radical SPPs of Four-Component Monomer Solids (Containing Monomer, Linker, DMPA, and EGDMA)

In a typical run, the four-component monomer cocrystal solid (**1·7**) prepared as described above was moulded using a mini-hand hydraulic press to form a monomer sheet with a rounded shape (diameter 7 mm and thickness 1 mm), and the sheet was put in a 4 mL glass vial. The vial was capped with a rubber septum and was degassed with an argon flow for 10 min. The sheet was then irradiated with UV light ($\lambda = 365$ nm) at room temperature for 24 h to obtain the four-component polymer sheet of P(**1·7**). The four-component monomer cocrystal solids (**1·6**, **2·6**, **3·6**, **4·6**, **5·6**, **2·7**, **3·7**, **4·7**, and **5·7**) were polymerized similarly.

For purification, the polymer sheets were washed (immersed) in a mixture of ethanol (10 mL) and toluene (10 mL) (50/50 v/v%), or DMF (20 mL), and sonicated (30 min) to fully remove the linkers and the unreacted monomers, DMPA, and EGDMA, giving purified polymer sheets, poly(4-vinyl pyridine) (P4VP) or poly(*N*-vinyl pyrrolidone) (PNVP) sheets, with the retained round shape as the final products.

**General Procedure for Free-Radical SPPs of Three-Component Monomer Solids
(Containing Monomer, Linker, and DMPA)**

The three-component monomer solids containing monomers (**6** and **7**), linkers (**1–5**), and photo-initiator DMPA were prepared and used for free-radical SPP in a similar manner as described above (Table S1).

Table S1 Free-radical SPPs of three-component solids (containing monomer, linker, and DMPA) at room temperature under UV irradiation ($\lambda = 365$ nm) for 24 h

Entry	Linker·M ^a	[M] ₀ /[Linker] ₀ /[DMPA] ₀ ^b	Monomer conversion (%)	M _p ^c	M _n ^c	\bar{D} ^c
1	1·6	2/1/0.03	91	16000	NA	NA
2	2·6	2/1/0.03	88	5900	NA	NA
3	3·6	1/1/0.03	89	5500	NA	NA
4	4·6	1/1/0.03	92	2200	NA	NA
5	5·6	4/1/0.03	99	93000	80000	1.64
6	1·7	2/1/0.03	91	7300	NA	NA
7	2·7	2/1/0.03	100	5000	NA	NA
8	3·7	1/1/0.03	100	5000	NA	NA
9	4·7	1/1/0.03	88	2100	NA	NA
10	5·7	4/1/0.03	97	42000	NA	NA

^a Combination of linker and monomer. ^b Polymerization in the solid phase under UV irradiation ($\lambda = 365$ nm) at room temperature for 24 h. ^c Polystyrene (PSt)-calibrated GPC values. DMF was used as the GPC eluent. M_p is the peak-top molecular weight. In most cases, the GPC baseline was not horizontal, hence, the M_n and \bar{D} values were not accurately determined, and we studied the M_p values instead.

Solution-Phase Free Radical Polymerization of Monomer (6** and **7**) (with EGDMA)
(Comparison Experiment)**

Monomer (**6** (42.0 mg, 0.4 mmol) or **7** (44.4 mg, 0.4 mmol)), DMPA (1.54 mg, 6.0 mmol), and EGDMA (31.7 mg, 0.16 mmol) were dissolved in dichloromethane (2 mL) in a glass vial,

which was capped and deoxygenated with an argon flow for 10 min. The obtained solutions in the vials were irradiated with UV light ($\lambda = 365$ nm) at room temperature for 24 h to generate covalently crosslinked polymers. The polymers were washed with a mixture of ethanol and toluene (50/50 v/v%) (4 mL) for 30 min to remove the unreacted monomers, DMPA, and EGDMA. The purified polymers were dried, yielding covalently crosslinked P4VP and PNVP as the final products, which were analyzed using PXRD (for P4VP and PNVP) and CM (for P4VP).

4. Stimuli-Responsive Emissive Polymer Sheets

Temperature. A covalently crosslinked four-component polymer sheet **P(5·6)** was covered with the aluminium foil and consequently heated from 22 °C (room temperature) to 30 °C, 50 °C, 70 °C, 100 °C, 120 °C, and 150 °C using a heater plate with the temperature controller. The polymer sheet was then cooled back to 22 °C. The polymer sheet was kept for 20 min at each temperature to ensure the well-distributed temperature on the sheet, and then immediately analyzed using CM.

pH. The polymer sheets **P(5·6)** were individually immersed in 4 mL vials containing pH-standard solutions with pH = 2.0, 7.0, and 11.0, and sonicated for 30 min. The polymer sheets were then taken out of the solutions, rinsed with CH₂Cl₂ to remove the residual ions adsorbed on the polymer surfaces, quickly dried with a nitrogen (N₂) flow, and analyzed using CM.

Solvent. The polymer sheets **P(5·6)** were immersed separately in 4 mL vials of toluene, *N,N*-dimethylformamide (DMF), ethanol (EtOH), 1,4-diodotetrafluorobenzene (I-C₆F₄-I, 0.1 M) dissolved in CH₂Cl₂, trifluoromethylbenzene (PhCF₃), and dichloromethane (CH₂Cl₂) and sonicated for 30 min. The polymer sheets were then taken out of the solutions, rinsed

with CH₂Cl₂ to remove the residual linker **5** adsorbed on the polymer surfaces, quickly dried with an N₂ flow, and analyzed using CM.

Host-Guest Interaction. The polymer sheet **P(5·6)** consecutively underwent reversible unloading-loading circles of different linkers **1–5**. The polymer sheet **P(5·6)** was first immersed in DMF (4 mL) with sonication (30 min) to completely remove linker **5**, subsequently re-immersed in a solution of linker **5** (0.05 M in CH₂Cl₂) with sonication for 30 min, to re-embed the linker **5**. Similarly, linkers **2**, **4**, **3**, and **1** were sequentially embedded and analyzed using CM for steps 1–12. After step 12, the purified P4VP polymer sheet was divided into two parts and re-embedded separately in two mixtures. Mixture 1 contained linkers **4** and **5** (0.05 M in CH₂Cl₂) (step 13) and mixture 2 contained all linkers **1–5** (0.05 M in CH₂Cl₂) (step 14). The re-embedded polymer sheets were then taken out of the solutions, rinsed with CH₂Cl₂ to remove the residual linker **5** adsorbed on the polymer surfaces, quickly dried with an N₂ flow, and analyzed using CM.

5. Raman spectra

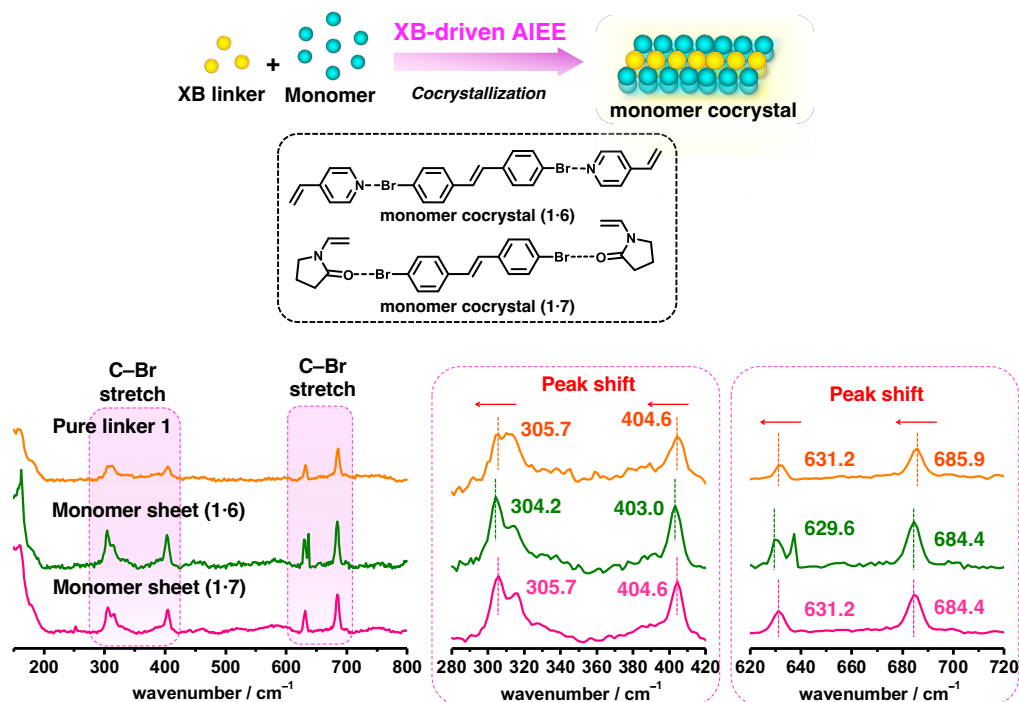


Fig. S1. Raman spectra of pure linker **1** (orange), monomer cocrystal solid (**1·6**) (green), and monomer cocrystal solid (**1·7**) (pink), and the zoom-in spectra for the C–Br stretching of the linker.

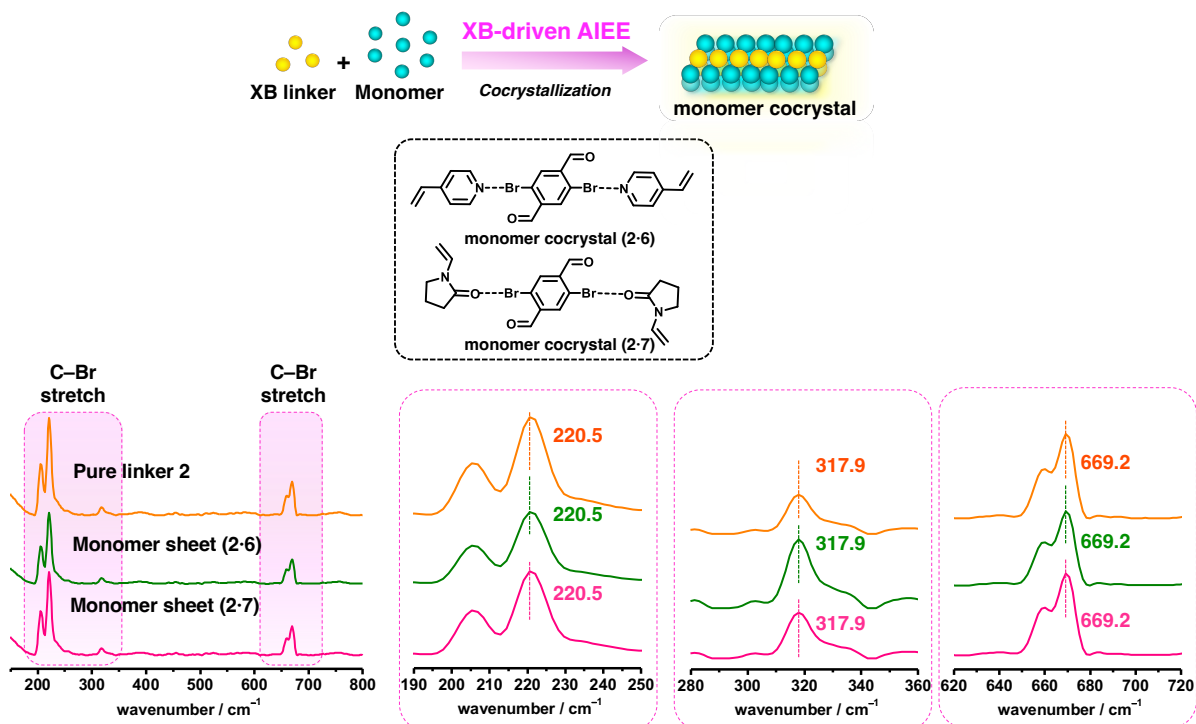


Fig. S2. Raman spectra of pure linker **2** (orange), monomer cocrystal solid (**2·6**) (green), and monomer cocrystal solid (**2·7**) (pink), and the zoom-in spectra for the C–Br stretching of the linker.

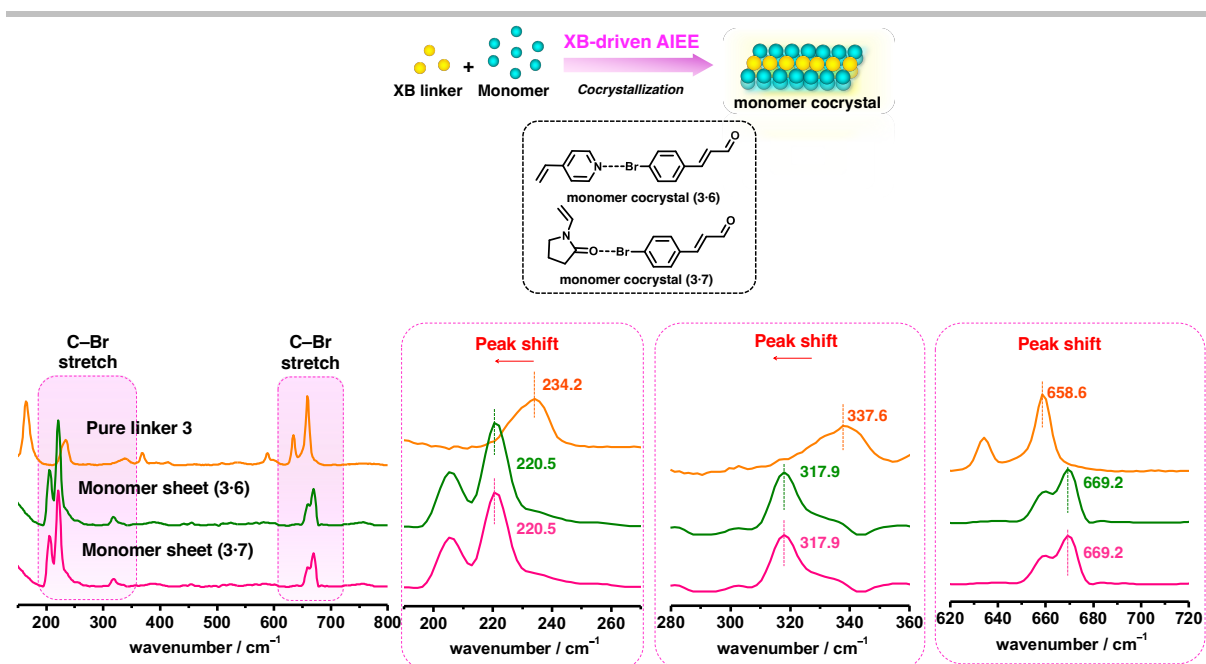


Fig. S3. Raman spectra of pure linker **3** (orange), monomer cocrystal solid (**3·6**) (green), and monomer cocrystal solid (**3·7**) (pink), and the zoom-in spectra for the C-Br stretching of the linker.

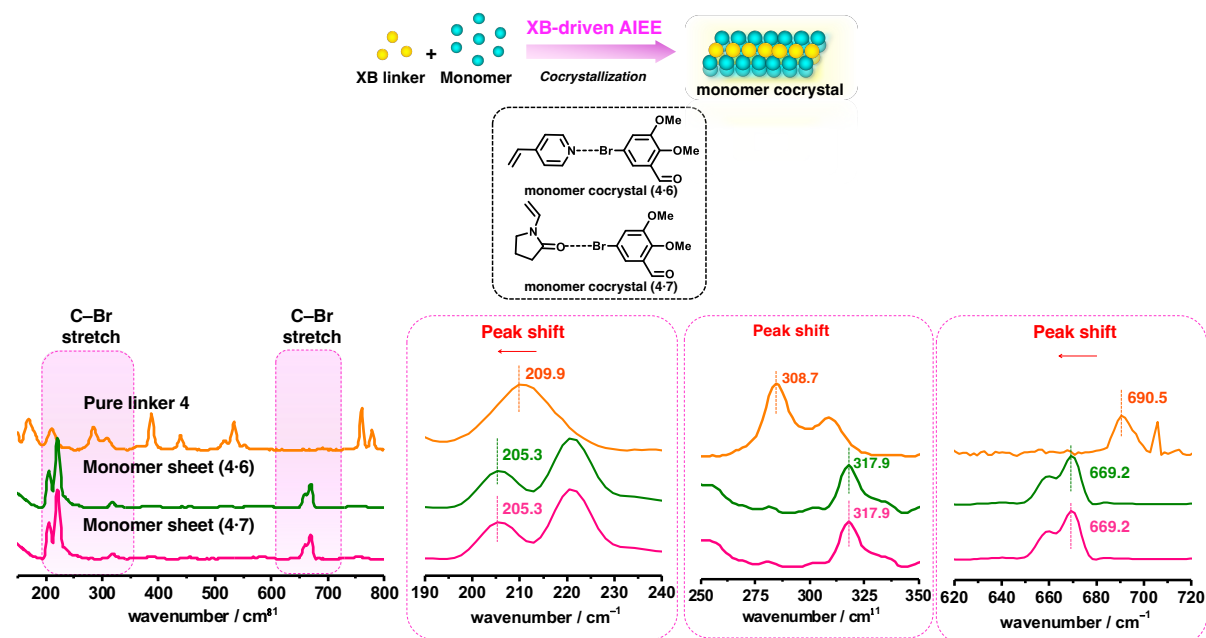


Fig. S4. Raman spectra of pure linker **4** (orange), monomer cocrystal solid (**4·6**) (green), and monomer cocrystal solid (**4·7**) (pink), and the zoom-in spectra for the C-Br stretching of the linker.

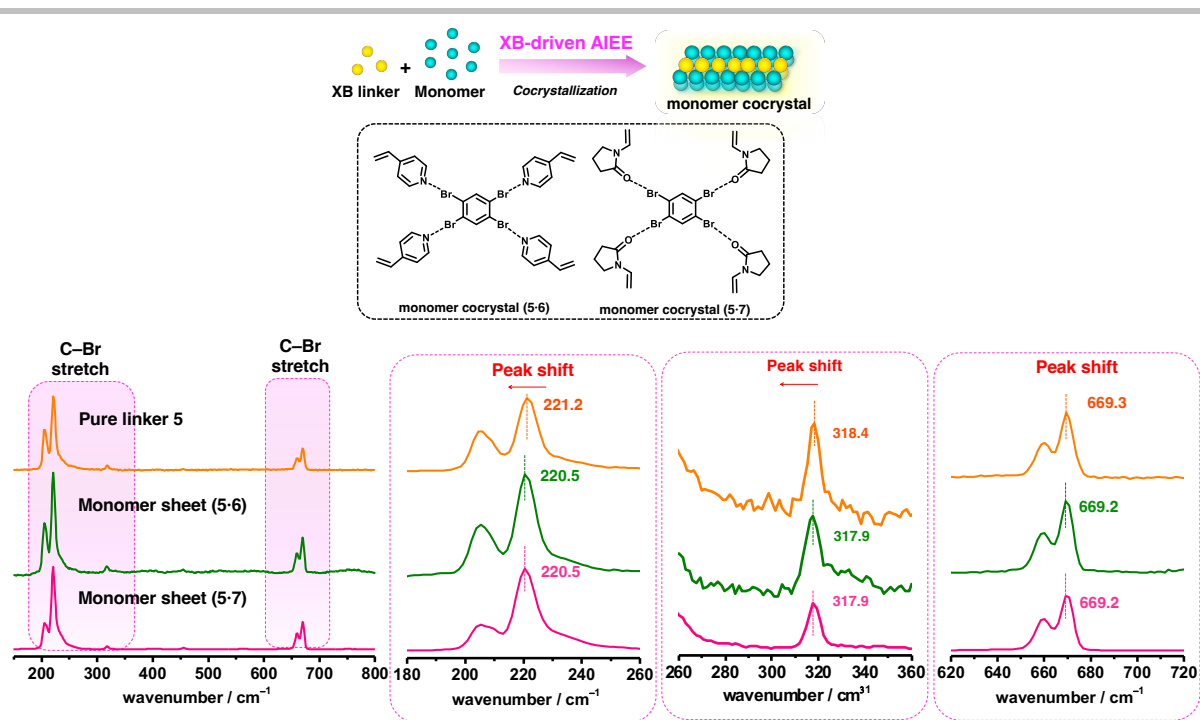


Fig. S5. Raman spectra of pure linker **5** (orange), monomer cocrystal solid (**5·6**) (green), and monomer cocrystal solid (**5·7**) (pink), and the zoom-in spectra for the C–Br stretching of the linker.

6. X-ray powder diffraction (PXRD) data

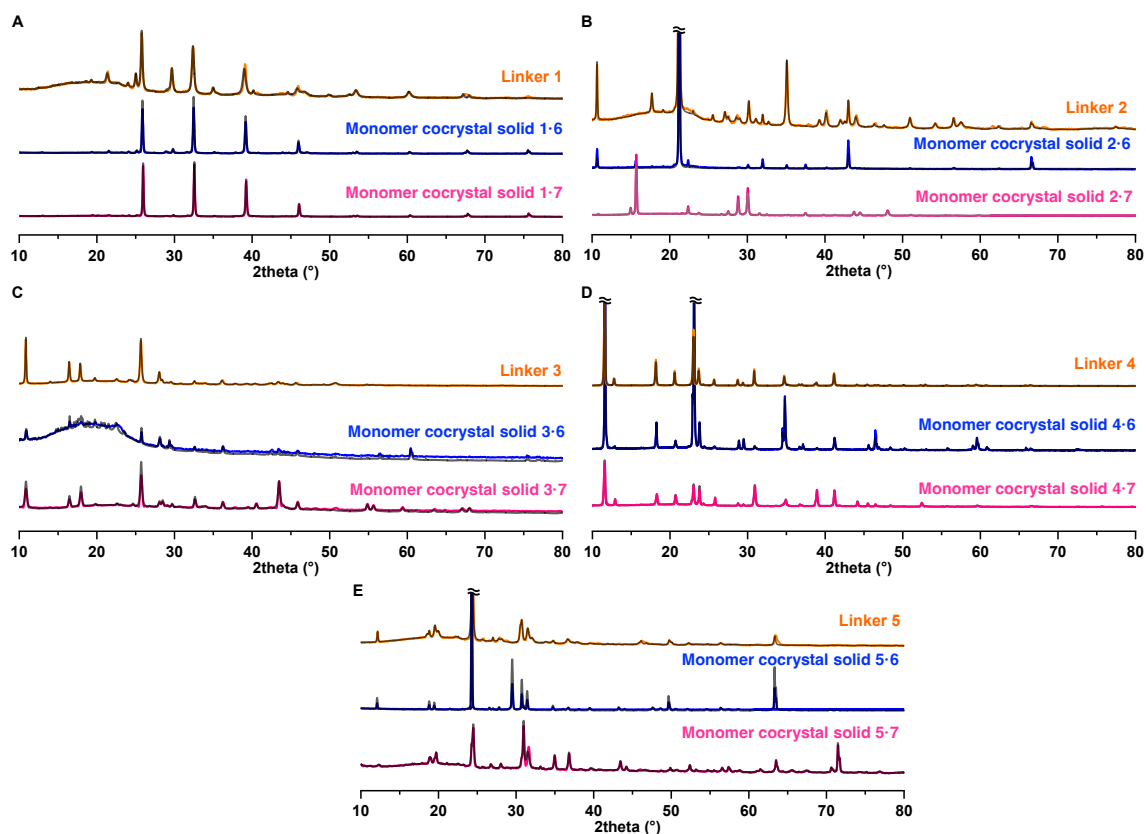


Fig. S6. Experimental PXRD patterns of pure linkers (orange), 4-component monomer cocrystal solids with monomer 6 (blue), 4-component monomer cocrystal solids with monomer 7 (pink), and their calculated PXRD patterns (grey) (overlapped with the experimental PXRD patterns). (A) pure linker 1, 4-component monomer cocrystal solids 1·6 and 1·7. (B) pure linker 2, 4-component monomer cocrystal solids 2·6 and 2·7. (C) pure linker 3, 4-component monomer cocrystal solids 3·6 and 3·7. (D) pure linker 4, 4-component monomer cocrystal solids 4·6 and 4·7. (E) pure linker 5, 4-component monomer cocrystal solids 5·6 and 5·7.

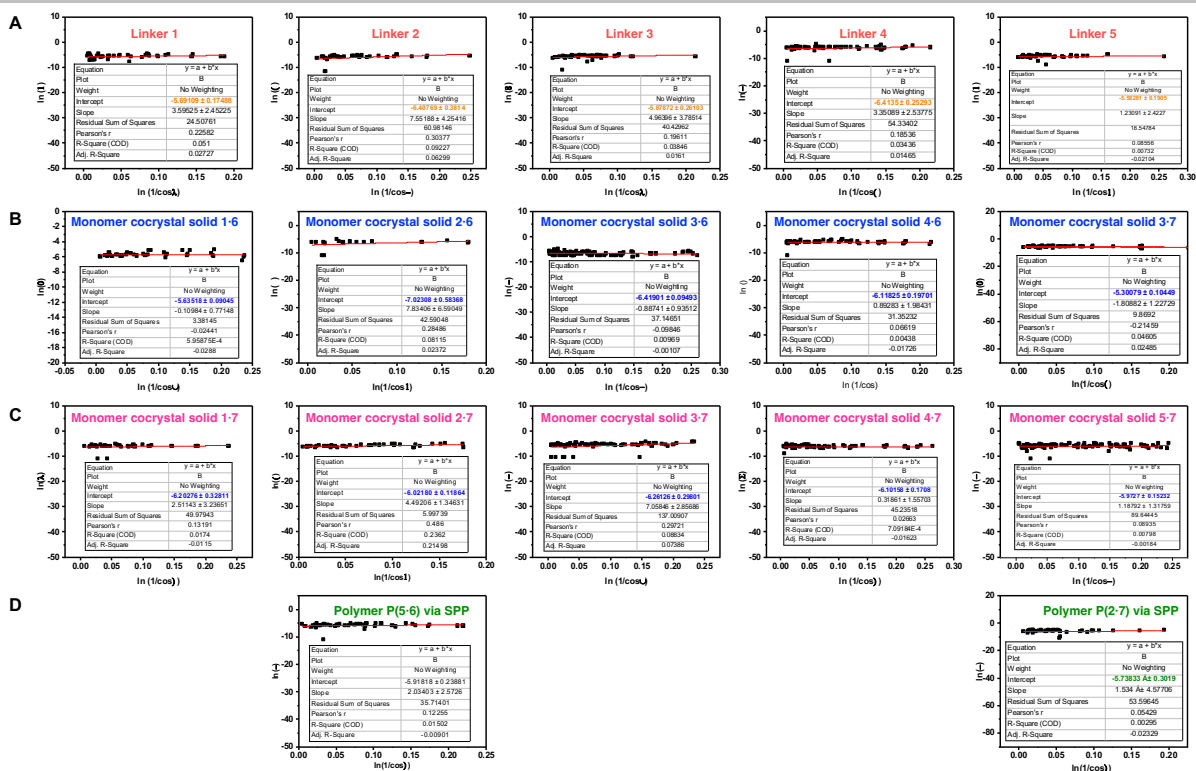


Fig. S7. Modified Scherrer equation fittings (least square method) for plots of $\ln(\beta)$ vs $\ln(1/\cos\theta)$ from experimental PXRD patterns (Figs. 2, S6, and S8; Equation (1); and Table S2). (A) pure linkers 1–5, (B) 4-component monomer cocrystal solids 1·6, 2·6, 3·6, 4·6, and 5·6, (C) 4-component monomer cocrystal solids 1·7, 2·7, 3·7, 4·7, and 5·7, and (D) polymers P(2·7) and P(5·6) obtained from free-radical SPP of the 4-component monomer cocrystal solids 2·7 and 5·6, respectively.

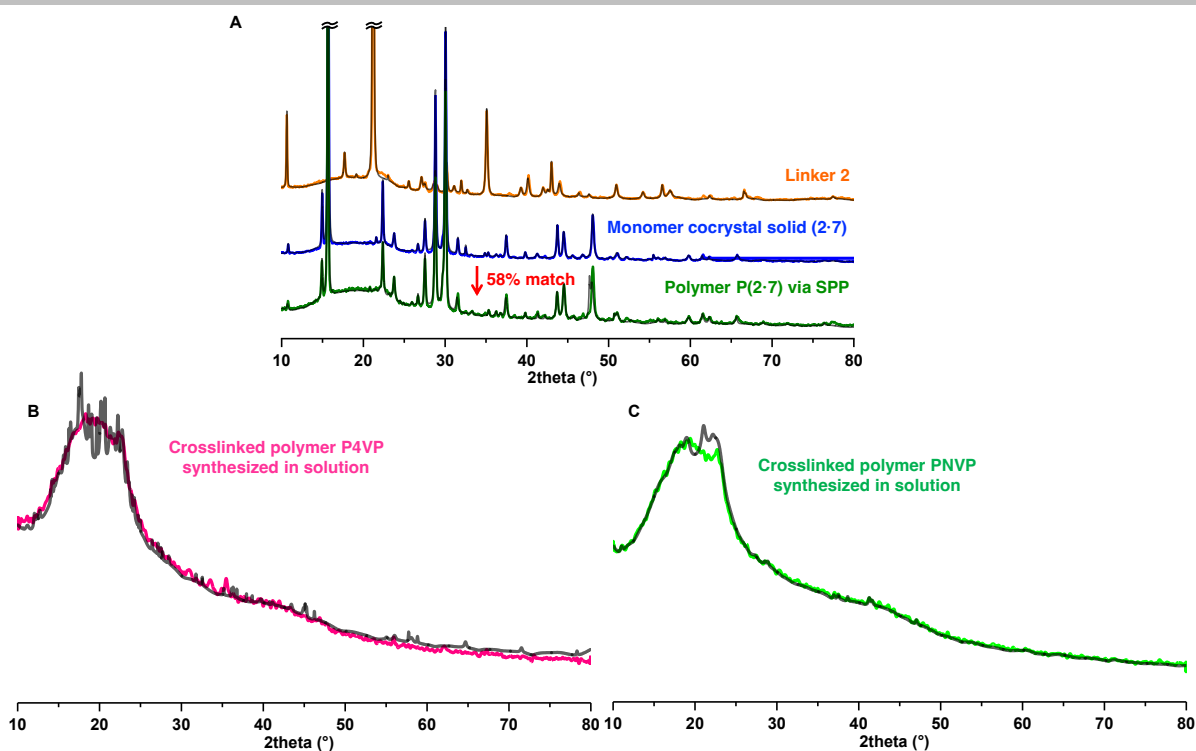


Fig. S8. Experimental PXRD patterns of (A) linker **2** (orange), 4-component monomer cocrystal solid **2·7** (blue), and polymer **P(2·7)** (green) obtained from free-radical SPP of the 4-component monomer cocrystal solid **2·7**, (B) crosslinked polymer P4VP synthesized in the solution phase (pink), and (C) crosslinked polymer PNVP synthesized in the solution phase (green) and their calculated PXRD patterns (grey) (overlapped with the experimental PXRD patterns).

Table S2 Powder X-ray diffraction (PXRD) data of pure linkers (1–5), 4-component monomer cocrystals of linkers (1–5) and monomers (6–7), and two presentative obtained polymers **P(5·6)** and **P(2·7)** (Figs. 2 and S6–S8)

Entry	Compound	2θ (°) ^a	FWHM (°) ^a	d_{hkl} spacing (nm) ^b	Microstrain (ϵ) ^c	Crystallite (grain) size (D) (nm) ^d	Dislocation density (\square) (nm ⁻²) ^e	R_p (%) ^f	Match ratio (%) ^g
1	XB linker 1	11.09	0.2891	0.797844	0.01299355	0.975911	1.049976	7.2	NA
		12.48	0.7110	0.709277	0.02837286				
		12.85	0.4909	0.688936	0.01902104				
		13.93	0.7110	0.635756	0.02539463				
		14.27	0.0468	0.620684	0.00163132				
		14.52	0.4061	0.610053	0.01390924				
		15.10	0.4298	0.586749	0.01414932				
		16.12	0.2370	0.549844	0.00730256				
		16.50	0.0790	0.537266	0.00237737				
		16.76	0.0790	0.528989	0.00233997				
		17.36	0.0790	0.510839	0.00225791				
		17.71	0.0790	0.500822	0.00221259				
		18.54	0.0790	0.478584	0.00211191				
		18.72	0.0790	0.474023	0.00209124				
		19.29	0.0790	0.460143	0.00202831				
		21.34	0.3243	0.416380	0.00751036				
		22.82	0.6848	0.389700	0.01480551				
		24.01	0.1815	0.370648	0.00372420				
		25.02	0.2138	0.355910	0.00420447				
		25.78	0.2312	0.345588	0.00440819				
		28.98	0.0790	0.308115	0.00133383				
		29.23	0.2765	0.305536	0.00462670				
		29.66	0.2765	0.301204	0.00455660				
		32.39	0.3208	0.276413	0.00481955				
		34.98	0.2863	0.256518	0.00396443				
		35.40	0.3950	0.253570	0.00540048				
		38.99	0.4384	0.231010	0.00540331				
		39.59	0.0318	0.227646	0.00038551				
		40.19	0.2404	0.224385	0.00286715				
		44.61	0.1720	0.203126	0.00182943				
		45.81	0.4514	0.198080	0.00466157				
		46.46	0.6741	0.195459	0.00685269				
		46.80	0.4678	0.194118	0.00471685				
		47.19	0.3311	0.192605	0.00330757				
49.84	0.2692	0.182967	0.00252816						
50.12	0.2498	0.182011	0.00233105						
52.53	0.3771	0.174214	0.00333436						
53.37	0.5282	0.171668	0.00458539						
60.01	0.2442	0.154164	0.00184517						
60.22	0.5378	0.153677	0.00404646						
67.20	0.2370	0.139311	0.00155646						
67.97	0.1975	0.137920	0.00127833						
2	XB linker 2	10.63	0.1093	0.832264	0.00512635	0.978576	1.044265	9.1	NA
		17.70	0.2057	0.501102	0.00576445				
		19.15	0.1975	0.463475	0.00510856				
		20.63	0.0007	0.430547	1.6782E-05				
		21.20	0.1296	0.419098	0.00302165				
		21.75	0.0007	0.408623	1.5898E-05				
		23.02	0.0790	0.386359	0.00169275				
		25.56	0.1901	0.348512	0.00365682				
		27.11	0.2603	0.328928	0.00471091				
		27.50	0.2843	0.324351	0.00506948				
		28.58	0.3053	0.312335	0.00522994				
		29.02	0.3412	0.307699	0.00575249				
		30.19	0.2169	0.296036	0.00350875				
		31.11	0.2346	0.287488	0.00367740				
		31.98	0.1580	0.279863	0.00240583				
		32.72	0.1580	0.273701	0.00234845				
		35.09	0.2463	0.255739	0.00339916				
		39.28	0.3026	0.229371	0.00369977				
		40.14	0.3231	0.224653	0.00385869				
		41.99	0.3372	0.215173	0.00383390				
		42.55	0.2524	0.212470	0.00282834				
43.02	0.1862	0.210257	0.00206147						
43.97	0.3411	0.205933	0.00368652						
46.36	0.1580	0.195858	0.00161005						
47.61	0.2370	0.191003	0.00234408						
50.95	0.3260	0.179239	0.00298557						

		54.21	0.1580	0.169205	0.00134693				
		56.57	0.2370	0.162694	0.00192175				
		57.52	0.4740	0.160231	0.00376830				
		62.36	0.2370	0.148908	0.00170886				
		66.54	0.1545	0.140532	0.00102744				
		66.75	0.3222	0.140141	0.00213413				
		77.45	0.3160	0.123235	0.00171950				
		10.84	0.1379	0.816188	0.00634172				
		13.99	0.1691	0.633043	0.00601355				
		16.44	0.1758	0.539213	0.00530998				
		17.86	0.1805	0.496649	0.00501221				
		19.73	0.2228	0.449979	0.00559032				
		22.32	0.0010	0.398315	2.2117E-05				
		22.52	0.3160	0.394823	0.00692543				
		24.12	0.1879	0.368983	0.00383741				
		24.34	0.2427	0.365697	0.00491042				
		24.63	0.1295	0.361457	0.0025883				
		25.67	0.2304	0.347044	0.00441241				
		28.05	0.2449	0.318115	0.00427788				
		28.42	0.1924	0.314057	0.00331525				
		28.96	0.4345	0.308323	0.00734133				
		29.54	0.3005	0.302400	0.00497315				
		30.76	0.2985	0.290679	0.00473498				
		32.58	0.2604	0.274845	0.00388805				
		33.05	0.1516	0.271043	0.00222955				
		33.38	0.3506	0.268438	0.00510226				
		33.90	0.4345	0.264439	0.0062205				
		36.11	0.3806	0.248746	0.00509441				
		37.64	0.0276	0.238979	0.00035335				
3	XB linker 3	37.85	0.3160	0.237701	0.00402145	0.97667	1.048343	5.7	NA
		39.23	0.3160	0.229652	0.00386894				
		39.41	0.3160	0.228644	0.00384981				
		40.22	0.0454	0.224225	0.00054103				
		40.36	0.3322	0.223479	0.00394386				
		40.62	0.3277	0.222108	0.00386334				
		41.79	0.2013	0.216157	0.00230074				
		42.21	0.4028	0.214103	0.00455361				
		42.37	0.3898	0.213331	0.00438839				
		42.54	0.2343	0.212518	0.00262619				
		43.36	0.4098	0.208687	0.00449784				
		43.95	0.3160	0.206022	0.00341697				
		44.10	0.1367	0.205356	0.0014726				
		44.45	0.3160	0.203820	0.00337446				
		45.61	0.3160	0.198902	0.00327926				
		46.21	0.3160	0.196458	0.00323179				
		49.24	0.2538	0.185055	0.00241657				
		50.23	0.2875	0.181638	0.00267615				
		50.53	0.3695	0.180630	0.00341614				
		50.84	0.4740	0.179601	0.00435173				
		54.77	0.2370	0.167607	0.00199627				
		55.50	0.1975	0.165574	0.00163793				
		72.28	0.1975	0.130720	0.00118003				
		11.57	0.1440	0.764850	0.00620183				
		12.12	0.0010	0.730262	4.11E-0500				
		12.79	0.1533	0.692155	0.00596806				
		17.67	0.0594	0.501946	0.00166747				
		18.18	0.1619	0.487979	0.00441527				
		20.60	0.1452	0.431167	0.00348623				
		20.90	0.0847	0.425046	0.0020038				
		22.42	0.2370	0.396561	0.00521785				
		23.02	0.1516	0.386359	0.00324837				
		23.70	0.1737	0.375425	0.00361216				
		24.29	0.0981	0.366439	0.00198901				
		25.46	0.1622	0.349858	0.00313280				
		25.69	0.1459	0.346778	0.00279189				
4	XB linker 4	28.73	0.1564	0.310739	0.00266462	0.978595	1.044224	10	NA
		29.40	0.1418	0.303808	0.00235842				
		30.85	0.1423	0.289851	0.00225033				
		31.09	0.1474	0.287668	0.00231208				
		34.44	0.0492	0.260415	0.00069265				
		34.72	0.1737	0.258379	0.00242442				
		35.20	0.4740	0.254965	0.00651984				
		36.62	0.1580	0.245398	0.00208335				
		36.99	0.1580	0.243028	0.00206101				
		38.69	0.1580	0.232732	0.00196369				
		38.88	0.1185	0.231638	0.00146499				
		41.15	0.1744	0.219369	0.00202720				
		41.70	0.0010	0.216602	1.1456E-05				
		41.84	0.1922	0.215910	0.00219386				
		44.09	0.1585	0.205400	0.00170787				

		45.42	0.1963	0.199690	0.00204657				
		46.38	0.1385	0.195778	0.00141066				
		46.79	0.1739	0.194158	0.00175386				
		48.31	0.1783	0.188398	0.00173473				
		50.11	0.1829	0.182045	0.00170715				
		52.31	0.1907	0.174895	0.00169438				
		52.90	0.0884	0.173082	0.00077532				
		53.05	0.1118	0.172628	0.00097735				
		55.64	0.2125	0.165191	0.00175712				
		58.37	0.1671	0.158098	0.00130539				
		58.55	0.1059	0.157655	0.00082425				
		59.24	0.1074	0.155983	0.00082425				
		59.45	0.2401	0.155482	0.00183484				
		59.77	0.3653	0.154726	0.00277360				
		59.93	0.0660	0.154351	0.00049950				
		60.72	0.1127	0.152530	0.00083950				
		60.88	0.1393	0.152168	0.00103433				
		65.78	0.1116	0.141970	0.00075299				
		65.96	0.1131	0.141626	0.00076049				
		66.42	0.1708	0.140757	0.00113844				
		66.59	0.1932	0.140439	0.00128358				
		68.34	0.3438	0.137263	0.00220983				
		72.58	0.1548	0.130254	0.00091984				
		12.15	0.1487	0.728466	0.00609639				
		18.53	0.2395	0.478840	0.00640607				
		18.81	0.1811	0.471775	0.00477061				
		19.55	0.2495	0.454081	0.00631904				
		19.96	0.3774	0.444846	0.00935810				
		22.23	0.2370	0.399907	0.00526360				
		22.53	0.2370	0.39465	0.00519171				
		24.34	0.1930	0.365697	0.00390486				
		25.62	0.3432	0.347710	0.00658592				
		27.02	0.1275	0.330003	0.00231547				
		27.77	0.3039	0.321259	0.00536420				
		28.15	0.2765	0.317008	0.00481200				
		30.54	0.2020	0.292722	0.00322846				
		30.73	0.2379	0.290956	0.00377757				
		31.51	0.3076	0.283929	0.00475734				
		32.07	0.5677	0.279098	0.00861866				
		32.28	0.0365	0.277330	0.00055033				
		33.85	0.3950	0.264818	0.00566386				
5	XB linker 5	34.78	0.2838	0.257947	0.00395387	0.97545	1.050969	12.9	NA
		36.66	0.4422	0.245139	0.00582392				
		37.34	0.3950	0.240830	0.00510069				
		37.70	0.0098	0.238612	0.00012525				
		37.89	0.3950	0.237460	0.00502110				
		39.51	0.4468	0.228089	0.00542841				
		41.83	0.1580	0.215959	0.00180396				
		42.46	0.1975	0.212900	0.00221829				
		45.89	0.2370	0.197754	0.00244272				
		46.11	0.2370	0.196861	0.00242972				
		46.81	0.1580	0.194079	0.00159274				
		49.75	0.2506	0.183277	0.00235833				
		50.05	0.3399	0.182249	0.00317688				
		52.24	0.3308	0.175112	0.00294372				
		52.42	0.1975	0.174553	0.00175055				
		54.70	0.2819	0.167805	0.00237803				
		56.37	0.3101	0.163223	0.00252505				
		63.34	0.5322	0.146838	0.00376431				
		79.03	0.1975	0.121163	0.00104484				
		12.94	0.1533	0.684165	0.00589829				
		19.37	0.1809	0.458260	0.00462503				
		21.54	0.1701	0.412559	0.00390185				
		23.20	0.2714	0.383402	0.00576900				
		24.10	0.1863	0.369284	0.00380799				
		25.15	0.1577	0.354100	0.00308469				
		25.88	0.1678	0.344275	0.00318658				
		28.84	0.1975	0.309578	0.00335146				
		29.81	0.1975	0.299722	0.00323758				
6	Monomer cocrystal (1-6)	31.61	0.1625	0.283054	0.00250486	0.975675	1.050484	9.4	NA
		32.47	0.1692	0.275751	0.00253537				
		35.13	0.1898	0.255457	0.00261623				
		35.59	0.2752	0.252260	0.00374113				
		37.83	0.2316	0.237822	0.00294904				
		39.17	0.1982	0.229990	0.00243068				
		40.78	0.1691	0.221274	0.00198505				
		43.93	0.2105	0.206111	0.00227732				
		44.76	0.1794	0.202480	0.00190105				
		45.98	0.1988	0.197387	0.00204453				
		46.38	0.3405	0.195778	0.00346810				

		47.03	0.3643	0.193223	0.00365312					
		52.48	0.2591	0.174368	0.00229351					
		52.98	0.1324	0.172840	0.00115920					
		53.15	0.1899	0.172327	0.00165647					
		53.49	0.2241	0.171312	0.00194038					
		58.75	0.3555	0.157166	0.00275568					
		60.27	0.1719	0.153561	0.00129209					
		60.42	0.2057	0.153216	0.00154150					
		61.17	0.3555	0.151516	0.00262444					
		67.40	0.2471	0.138947	0.00161666					
		67.72	0.1763	0.138368	0.00114650					
		67.91	0.1565	0.138027	0.00101410					
		68.18	0.395	0.137546	0.00254657					
		75.30	0.0941	0.126210	0.00053220					
		75.56	0.1460	0.125840	0.00082187					
		75.77	0.1716	0.125544	0.00096233					
		10.65	0.1266	0.830706	0.00592654					
		15.63	0.1379	0.566970	0.00438400					
		20.58	0.0010	0.431582	2.4034E-05					
		21.23	0.1259	0.418513	0.00293114					
		21.79	0.0010	0.407882	2.2669E-05					
		22.37	0.0913	0.397436	0.00201469					
		28.98	0.4175	0.308115	0.00704902					
		30.10	0.1877	0.296900	0.00304590					
7	Monomer cocystal (2-6)	31.97	0.1433	0.279948	0.00218271	0.980435	1.040309	10.6	NA	
		35.08	0.1550	0.255809	0.00213979					
		37.51	0.1478	0.239777	0.00189927					
		40.20	0.1288	0.224332	0.00153573					
		43.01	0.1652	0.210304	0.00182944					
		56.58	0.1370	0.162667	0.00111065					
		56.73	0.1308	0.162273	0.00105707					
		62.38	0.2212	0.148865	0.00159431					
		66.59	0.1213	0.140439	0.00080589					
		66.78	0.1265	0.140085	0.00083741					
		10.21	0.2307	0.866404	0.01126784					
		10.89	0.2003	0.812452	0.00916881					
		11.17	0.0790	0.792148	0.00352505					
		11.56	0.0647	0.765509	0.00278894					
		11.80	0.1096	0.749993	0.00462764					
		12.08	0.1037	0.732671	0.00427631					
		12.51	0.1304	0.707583	0.00519111					
		14.74	0.1111	0.600997	0.00374785					
		15.02	0.0790	0.589856	0.00261475					
		15.43	0.0790	0.574273	0.00254446					
		15.59	0.0790	0.568416	0.00251802					
		15.83	0.1185	0.559851	0.00371905					
		16.03	0.0395	0.552911	0.00122402					
		16.50	0.1185	0.537266	0.00356606					
		17.05	0.0790	0.520057	0.00229959					
		17.37	0.0790	0.510547	0.00225659					
		17.59	0.1580	0.504211	0.00445586					
		17.72	0.3950	0.500541	0.01105662					
		17.98	0.2370	0.493362	0.00653648					
		18.16	0.1185	0.488512	0.00323531					
		18.49	0.0395	0.479867	0.00105886					
		18.82	0.1185	0.471526	0.00311989					
		19.04	0.0395	0.466127	0.00102773					
8	Monomer cocystal (3-6)	19.76	0.1975	0.449303	0.00494784	0.978614	1.044185	6.5	NA	
		20.55	0.1185	0.432205	0.00285224					
		20.80	0.1975	0.427067	0.00469534					
		21.00	0.1185	0.423044	0.00278977					
		21.50	0.1975	0.413318	0.00453900					
		22.48	0.4740	0.395516	0.01040711					
		23.49	0.1185	0.378734	0.00248692					
		23.65	0.0395	0.376208	0.00082320					
		25.75	0.0790	0.345984	0.00150807					
		26.91	0.0395	0.331327	0.00072039					
		28.12	0.2765	0.317339	0.00481735					
		28.52	0.0790	0.312979	0.00135628					
		29.04	0.0395	0.307492	0.00066547					
		29.35	0.1185	0.304314	0.00197440					
		29.63	0.1185	0.301502	0.00195490					
		31.98	0.0790	0.279863	0.00120291					
		32.61	0.1580	0.274599	0.00235682					
		33.13	0.0395	0.270407	0.00057943					
		33.57	0.0395	0.266962	0.00057140					
		33.80	0.0395	0.265198	0.00056727					
		33.96	0.0395	0.263985	0.00056444					
		34.14	0.1185	0.262635	0.00168385					
		34.77	0.0395	0.258019	0.00055048					

		34.95	0.0395	0.256731	0.00054746				
		35.10	0.0790	0.255668	0.00108994				
		36.25	0.1975	0.247817	0.00263266				
		36.94	0.0790	0.243345	0.00103200				
		39.05	0.0790	0.230669	0.00097206				
		39.75	0.1821	0.226767	0.00219795				
		40.35	0.1502	0.223532	0.00178365				
		41.89	0.1356	0.215664	0.00154578				
		42.24	0.0637	0.213958	0.00071956				
		42.43	0.2148	0.213043	0.00241448				
		42.93	0.0883	0.210677	0.00097985				
		43.32	0.1580	0.208871	0.00173593				
		43.61	0.0395	0.207549	0.00043080				
		44.08	0.0790	0.205444	0.00085146				
		44.40	0.0790	0.204038	0.00084467				
		44.58	0.0395	0.203255	0.00042044				
		44.74	0.0790	0.202566	0.00083756				
		45.80	0.1185	0.198121	0.00122404				
		45.91	0.1185	0.197672	0.00122077				
		46.88	0.0395	0.193806	0.00039752				
		47.98	0.0395	0.189616	0.00038729				
		48.57	0.0395	0.187450	0.00038198				
		50.36	0.0395	0.181199	0.00036660				
		50.76	0.0790	0.179865	0.00072660				
		52.89	0.0395	0.173113	0.00034652				
		54.06	0.0395	0.169639	0.00033782				
		54.91	0.0395	0.167213	0.00033172				
		56.44	0.0790	0.163038	0.00064233				
		56.60	0.0395	0.162615	0.00032009				
		56.89	0.0395	0.161854	0.00031816				
		57.43	0.0790	0.160460	0.00062922				
		57.71	0.1185	0.159748	0.00093838				
		60.43	0.1483	0.153193	0.00111113				
		60.61	0.1771	0.152781	0.00132213				
		60.93	0.0194	0.152055	0.00014391				
		61.13	0.1176	0.151605	0.00086886				
		62.41	0.0395	0.148800	0.00028453				
		66.55	0.0790	0.140513	0.00052526				
		66.88	0.0790	0.139900	0.00052198				
		68.31	0.0794	0.137316	0.00051064				
		73.52	0.0790	0.128819	0.00046144				
		75.43	0.1289	0.126025	0.00072731				
		75.65	0.1634	0.125713	0.00091832				
		76.78	0.1484	0.124142	0.00081726				
		77.04	0.2198	0.123788	0.00120484				
		77.54	0.1619	0.123114	0.00087955				
		78.08	0.0790	0.122398	0.00042507				
		79.14	0.0395	0.121022	0.00020856				
		11.64	0.1194	0.760266	0.00511121				
		11.84	0.0010	0.747468	4.2079E-05				
		12.13	0.1580	0.729663	0.00648843				
		12.89	0.0790	0.686807	0.00305146				
		16.31	0.1975	0.543482	0.00601363				
		18.26	0.1307	0.485859	0.00354852				
		20.71	0.1754	0.428902	0.00418846				
		22.39	0.1406	0.397086	0.00309974				
		22.92	0.0864	0.388022	0.00185961				
		23.11	0.1296	0.384875	0.00276586				
		23.81	0.1474	0.373716	0.00305066				
		24.42	0.1255	0.364517	0.00253060				
		25.70	0.2720	0.346645	0.00520280				
		28.89	0.1327	0.309054	0.00224778				
		29.50	0.1334	0.302801	0.00221085				
		30.92	0.1496	0.289211	0.00236015				
9	Monomer cocrystal (4-6)	31.15	0.1492	0.287128	0.00233558	0.977574	1.046407	8.6	NA
		34.54	0.1269	0.259684	0.00178103				
		34.82	0.1602	0.257660	0.00222916				
		35.30	0.1459	0.254265	0.00200079				
		36.71	0.1557	0.244817	0.00204763				
		37.14	0.1400	0.242081	0.00181830				
		38.94	0.2998	0.231295	0.00370019				
		41.22	0.1928	0.219013	0.00223692				
		41.83	0.1998	0.215959	0.00228121				
		42.13	0.3110	0.214491	0.00352314				
		42.50	0.2765	0.212709	0.00310240				
		45.59	0.1346	0.198985	0.00139748				
		46.44	0.2345	0.195539	0.00238500				
		46.89	0.4121	0.193767	0.00414629				
		48.40	0.2012	0.188069	0.00195342				
		49.71	0.1545	0.183415	0.00145529				

		50.23	0.2333	0.181638	0.00217164				
		52.43	0.1580	0.174523	0.00140013				
		53.00	0.0790	0.172779	0.00069137				
		55.77	0.1462	0.164836	0.00120558				
		59.04	0.1277	0.156463	0.00098404				
		59.20	0.0884	0.156078	0.00067899				
		59.56	0.1486	0.155221	0.00113307				
		59.75	0.1360	0.154773	0.00103302				
		60.84	0.1147	0.152258	0.00085235				
		60.97	0.1973	0.151965	0.00146237				
		65.88	0.0790	0.141779	0.00053201				
		66.06	0.0790	0.141436	0.00053019				
		66.48	0.1580	0.140644	0.00105192				
		66.66	0.1975	0.140308	0.00131040				
		72.38	0.0656	0.130564	0.00039123				
		72.64	0.1355	0.130161	0.00080427				
		12.10	0.1333	0.731465	0.00548778				
		17.60	0.3235	0.503927	0.00911796				
		18.51	0.2575	0.479353	0.00689510				
		18.79	0.182	0.472272	0.00479952				
		19.48	0.2489	0.455697	0.00632694				
		19.92	0.3552	0.445730	0.00882568				
		22.05	0.5802	0.403131	0.01299368				
		22.40	0.4581	0.396911	0.01009487				
		22.96	0.2365	0.387355	0.00508116				
		24.30	0.1814	0.366290	0.00367639				
		25.68	0.1239	0.346911	0.00237186				
		26.49	0.3000	0.336484	0.00556129				
		27.03	0.1161	0.329883	0.00210763				
		27.79	0.2919	0.321032	0.00514852				
		28.25	0.5193	0.315908	0.00900419				
		28.58	0.2728	0.312335	0.00467320				
		28.74	0.4579	0.310633	0.00779851				
		30.50	0.1850	0.293097	0.00296083				
		30.70	0.2185	0.291233	0.00347308				
		31.46	0.2867	0.284369	0.00444152				
		31.98	0.5739	0.279863	0.00873863				
		33.85	0.4710	0.264818	0.00675362				
		34.31	0.0870	0.261372	0.00122974				
10	Monomer cocrystal (5-6)	34.67	0.4375	0.258740	0.00611578	0.974161	1.05375	9.0	NA
		36.52	0.2370	0.246047	0.00313419				
		37.25	0.2370	0.241391	0.00306836				
		37.61	0.2370	0.239163	0.00303680				
		37.79	0.2370	0.238065	0.00302124				
		38.02	0.2961	0.236677	0.00375006				
		39.43	0.2370	0.228533	0.00288577				
		39.81	0.2370	0.226439	0.00285591				
		40.20	0.2892	0.224332	0.00344823				
		41.82	0.2370	0.216009	0.00270664				
		43.25	0.4384	0.209192	0.00482523				
		45.59	0.2370	0.198985	0.00246065				
		45.96	0.2370	0.197469	0.00243857				
		46.36	0.2370	0.195858	0.00241508				
		46.70	0.2370	0.194511	0.00239541				
		49.74	0.1807	0.183312	0.00170091				
		49.93	0.5181	0.182659	0.00485570				
		56.34	0.2786	0.163303	0.00226998				
		63.37	0.2187	0.146776	0.00154598				
		63.54	0.3386	0.146424	0.00238562				
		63.76	0.0647	0.145972	0.00045390				
		63.89	0.3923	0.145706	0.00274520				
		74.18	0.1185	0.127836	0.00068392				
		78.16	0.1975	0.122292	0.00106115				
		12.09	0.1588	0.732068	0.00654302				
		17.63	0.1805	0.503076	0.00507866				
		17.82	0.0763	0.497755	0.00212357				
		18.43	0.3036	0.481416	0.00816543				
		18.75	0.2268	0.473271	0.00599393				
		19.49	0.2730	0.455466	0.00693593				
		19.88	0.3938	0.446618	0.00980486				
		21.79	0.4740	0.407882	0.01074514				
11	Polymer P(5-6)	21.99	0.0719	0.404217	0.00161472	0.976107	1.049554	10.1	55% (31/56)
		22.25	0.5394	0.399552	0.01196863				
		22.75	0.2302	0.390883	0.00499269				
		24.29	0.1935	0.366439	0.00392329				
		26.45	0.3139	0.336984	0.00582808				
		27.76	0.4007	0.321372	0.00707548				
		28.21	0.2634	0.316347	0.00457386				
		30.48	0.2159	0.293285	0.00345775				
		30.66	0.2240	0.291604	0.00356538				

		31.43	0.3214	0.284634	0.00498409				
		31.94	0.4756	0.280204	0.00725140				
		33.55	0.2237	0.267117	0.00323802				
		33.91	0.2498	0.264363	0.00357513				
		34.22	0.3243	0.262039	0.00459676				
		34.37	0.2405	0.260930	0.00339314				
		34.53	0.2502	0.259757	0.00351261				
		34.66	0.4389	0.258812	0.00613724				
		36.48	0.5925	0.246307	0.00784468				
		37.20	0.2993	0.241704	0.00388053				
		37.36	0.0012	0.240705	1.5487E-05				
		37.56	0.1975	0.239470	0.00253429				
		37.78	0.0033	0.238126	4.208E-050				
		40.60	0.1185	0.222213	0.00139778				
		45.74	0.1975	0.198367	0.00204305				
		46.33	0.2370	0.195977	0.00241683				
		48.31	0.1185	0.188398	0.00115292				
		49.67	0.2370	0.183554	0.00223443				
		50.07	0.2370	0.182181	0.00221412				
		52.11	0.2370	0.175519	0.00211508				
		56.30	0.3173	0.163410	0.00258747				
		63.25	0.3160	0.147025	0.00223903				
		69.01	0.5490	0.136093	0.00348477				
		13.02	0.1852	0.679979	0.00708150				
		19.45	0.1226	0.456393	0.00312135				
		20.17	0.1876	0.440261	0.00460234				
		21.47	0.3305	0.413889	0.00760651				
		23.35	0.1708	0.380973	0.00360663				
		24.15	0.1486	0.368531	0.00303092				
		25.15	0.2091	0.354100	0.00409009				
		25.96	0.1438	0.343232	0.00272210				
		26.41	0.0012	0.337485	2.2315E-05				
		28.92	0.3042	0.308740	0.00514720				
		29.86	0.1766	0.299232	0.00288990				
		31.70	0.1919	0.282271	0.00294921				
		32.56	0.1597	0.275009	0.00238604				
		33.08	0.0012	0.270804	1.7631E-05				
		35.17	0.1862	0.255175	0.00256350				
		37.85	0.3555	0.237701	0.00452413				
		38.52	0.2765	0.233720	0.00345283				
12	Monomer cocrystal solid 1·7	39.24	0.1975	0.229596	0.00241742	0.977876	1.04576	9.4	NA
		40.31	0.2370	0.223745	0.00281745				
		40.84	0.1185	0.220963	0.00138883				
		43.93	0.1503	0.206111	0.00162604				
		44.42	0.1398	0.203950	0.00149400				
		46.06	0.1861	0.197063	0.00191020				
		46.44	0.3035	0.195539	0.00308677				
		47.09	0.1415	0.192990	0.00141690				
		50.31	0.3090	0.181368	0.00287106				
		52.57	0.1648	0.174091	0.00145590				
		53.08	0.1842	0.172538	0.00160921				
		53.56	0.2211	0.171104	0.00191150				
		60.35	0.1580	0.153377	0.00118571				
		60.52	0.1462	0.152987	0.00109342				
		67.46	0.1834	0.138838	0.00119854				
		67.80	0.1762	0.138224	0.00114412				
		67.99	0.1692	0.137884	0.00109474				
		75.63	0.1493	0.125741	0.00083938				
		75.84	0.1663	0.125445	0.00093143				
		10.81	0.1345	0.818446	0.00620263				
		14.97	0.1315	0.591815	0.00436710				
		15.69	0.1419	0.564815	0.00449369				
		18.25	0.1580	0.486123	0.00429211				
		21.58	0.1044	0.411804	0.00239024				
		22.37	0.1490	0.397436	0.00328794				
		23.77	0.2139	0.374336	0.00443465				
		26.67	0.1506	0.334254	0.00277223				
		27.54	0.1818	0.323889	0.00323686				
		28.82	0.1770	0.309789	0.00300576				
13	Monomer cocrystal (2·7)	29.65	0.0894	0.301303	0.00147379	0.977219	1.047167	6.9	NA
		30.06	0.1929	0.297286	0.00313465				
		31.56	0.1654	0.283491	0.00255381				
		32.52	0.1006	0.275338	0.00150499				
		34.87	0.1722	0.257302	0.00239248				
		35.27	0.1620	0.254475	0.00222359				
		36.26	0.1145	0.247751	0.00152582				
		37.48	0.2040	0.239962	0.00262371				
		39.8	0.1832	0.226493	0.00220821				
		41.22	0.2568	0.219013	0.00297947				
		43.74	0.2118	0.206962	0.00230238				

		44.51	0.2501	0.203559	0.00266675				
		45.57	0.2736	0.199067	0.00284203				
		46.82	0.2584	0.194040	0.00260421				
		48.06	0.2782	0.189319	0.00272257				
		50.20	0.4278	0.181739	0.00398483				
		50.86	0.2083	0.179535	0.00191151				
		51.02	0.4177	0.179009	0.00381936				
		52.29	0.2691	0.174957	0.00239202				
		55.49	0.0934	0.165602	0.00077476				
		55.65	0.1026	0.165163	0.00084820				
		56.06	0.2709	0.164052	0.00222026				
		56.94	0.1580	0.161724	0.00127131				
		59.80	0.3910	0.154655	0.00296693				
		61.43	0.3812	0.150937	0.00279964				
		62.34	0.4730	0.148951	0.00341185				
		65.74	0.3927	0.142047	0.00265168				
		65.96	0.1064	0.141626	0.00071544				
		10.71	0.2780	0.826066	0.01294071				
		14.93	0.1495	0.593391	0.00497834				
		15.66	0.1519	0.565890	0.00481971				
		20.79	0.1049	0.427270	0.00249511				
		22.38	0.1899	0.397261	0.00418855				
		23.76	0.2418	0.374491	0.00501525				
		24.49	0.0900	0.363491	0.00180942				
		24.62	0.0955	0.361601	0.00190955				
		24.92	0.4076	0.357316	0.00804884				
		26.68	0.1638	0.334131	0.00301405				
		27.53	0.1956	0.324005	0.00348388				
		28.80	0.2150	0.309999	0.00365371				
		29.31	0.0010	0.304720	1.6685E-050				
		29.69	0.3085	0.300906	0.00507857				
		30.04	0.2101	0.297480	0.00341653				
		31.47	0.2568	0.284281	0.00397698				
		33.33	0.1843	0.268830	0.00268637				
		35.33	0.1466	0.254056	0.00200856				
		36.21	0.2312	0.248082	0.00308552				
		36.75	0.2069	0.244559	0.00271779				
14	Polymer P(2-7)	37.43	0.3035	0.240271	0.00390901	0.976825	1.048013	8.5	58 % (28/48)
		39.82	0.1920	0.226384	0.00231302				
		41.34	0.1881	0.218405	0.00217547				
		42.23	0.3570	0.214006	0.00403375				
		43.70	0.2415	0.207142	0.00262789				
		44.54	0.2848	0.203429	0.00303448				
		45.74	0.3080	0.198367	0.00318612				
		46.70	0.2144	0.194511	0.00216699				
		47.43	0.0492	0.191686	0.00048870				
		47.67	0.1580	0.190777	0.00156051				
		47.96	0.4175	0.189691	0.00409542				
		50.70	0.1329	0.180064	0.00122399				
		51.04	0.4030	0.178944	0.00368329				
		52.75	0.3496	0.173539	0.00307630				
		56.03	0.2019	0.164133	0.00165579				
		56.89	0.1185	0.161854	0.00095448				
		59.80	0.4356	0.154655	0.00330536				
		61.49	0.3160	0.150804	0.00231803				
		62.32	0.1975	0.148994	0.00142517				
		65.38	0.1241	0.142741	0.00084378				
		65.66	0.2370	0.142200	0.00160278				
		71.88	0.1580	0.131349	0.00095098				
		73.10	0.1580	0.129455	0.00092998				
		10.86	0.2662	0.814689	0.01221927				
		11.47	0.0020	0.771496	8.6893E-05				
		11.90	0.2187	0.743713	0.00915602				
		13.89	0.1958	0.637578	0.00701368				
		14.74	0.2646	0.600997	0.00892602				
		16.47	0.2294	0.538238	0.00691616				
		17.43	0.0020	0.508803	5.6929E-05				
		17.95	0.2590	0.494179	0.00715538				
		19.80	0.2849	0.448404	0.00712270				
15	Monomer cocrystal (3-7)	20.27	0.5999	0.438112	0.01464307	0.978081	1.045323	7.3	NA
		22.63	0.2671	0.392929	0.00582454				
		23.05	0.2523	0.385863	0.00539887				
		24.67	0.2375	0.360880	0.00473894				
		25.19	0.0020	0.353547	3.9057E-05				
		25.71	0.2421	0.346513	0.00462902				
		26.22	0.0020	0.339887	3.7471E-05				
		26.79	0.1254	0.332784	0.00229763				
		28.07	0.2496	0.317893	0.00435674				
		28.48	0.2595	0.313409	0.00446164				
		29.04	0.2867	0.307492	0.00483017				

		29.71	0.2024	0.300708	0.00332959				
		30.52	0.4883	0.292910	0.00780962				
		32.13	0.0020	0.278590	3.0304E-05				
		32.65	0.2507	0.274271	0.00373475				
		33.14	0.3160	0.270327	0.00463399				
		33.50	0.1575	0.267504	0.00228339				
		33.88	0.6674	0.264590	0.00956079				
		36.24	0.3160	0.247883	0.00421349				
		37.63	0.4740	0.239040	0.00607013				
		39.13	0.3160	0.230216	0.00387965				
		39.50	0.2765	0.228144	0.00336027				
		40.03	0.1975	0.225245	0.00236573				
		40.56	0.3160	0.222423	0.00373141				
		42.15	0.3555	0.214394	0.00402516				
		42.97	0.1185	0.210490	0.00131363				
		43.48	0.3160	0.208139	0.00345777				
		43.98	0.4740	0.205888	0.00512159				
		44.52	0.3555	0.203515	0.00378966				
		45.89	0.3160	0.197754	0.00325696				
		46.85	0.3950	0.193923	0.00397804				
		47.96	0.4345	0.189691	0.00426218				
		49.38	0.2765	0.184563	0.00262424				
		50.47	0.4345	0.180830	0.00402254				
		51.49	0.2765	0.177485	0.00250181				
		52.19	0.2370	0.175268	0.00211134				
		54.38	0.2370	0.168716	0.00201302				
		54.87	0.3160	0.167325	0.00265602				
		55.64	0.3160	0.165191	0.00261293				
		58.20	0.2765	0.158520	0.00216758				
		59.40	0.3160	0.155601	0.00241731				
		59.95	0.1975	0.154304	0.00149411				
		60.53	0.0020	0.152964	1.4955E-05				
		61.07	0.4603	0.151740	0.00340489				
		62.32	0.9480	0.148994	0.00684083				
		63.42	0.4618	0.146672	0.00326126				
		64.19	0.1730	0.145097	0.00120358				
		64.75	0.4826	0.143977	0.00332132				
		65.36	0.5094	0.142780	0.00346483				
		67.04	0.3505	0.139605	0.00230884				
		68.00	0.2917	0.137866	0.00188698				
		68.66	0.1531	0.136701	0.00097819				
		70.08	0.2788	0.134275	0.00173476				
		70.99	0.5541	0.132776	0.00339014				
		74.76	0.9480	0.126987	0.00541414				
		75.23	0.9480	0.126310	0.00536836				
		11.58	0.1816	0.764192	0.00781440				
		12.73	0.0083	0.695403	0.00032466				
		12.93	0.1371	0.684692	0.00527911				
		13.84	0.1755	0.639870	0.00630946				
		15.73	0.3361	0.563388	0.01061622				
		16.21	0.0938	0.546812	0.00287395				
		16.37	0.3098	0.541503	0.00939798				
		18.31	0.2019	0.484543	0.00546638				
		20.71	0.1860	0.428902	0.00444159				
		22.58	0.2765	0.393787	0.00604323				
		22.80	0.0673	0.390037	0.00145635				
		23.04	0.1836	0.386028	0.00393054				
		23.60	0.0932	0.376994	0.00194658				
		23.80	0.1275	0.373871	0.00263995				
		24.05	0.1185	0.370041	0.00242734				
		24.30	0.1580	0.366290	0.00320215				
		25.52	0.2370	0.349049	0.00456640				
16	Monomer cocrystal (4-7)	25.82	0.0790	0.345061	0.00150384	0.977514	1.046536	11.3	NA
		28.78	0.1464	0.310210	0.00248973				
		29.45	0.1340	0.303304	0.00222473				
		30.94	0.2089	0.289029	0.00329345				
		32.61	0.2704	0.274599	0.00403344				
		33.65	0.2919	0.266346	0.00421190				
		34.39	0.1019	0.260782	0.00143679				
		34.51	0.2648	0.259903	0.00371988				
		34.75	0.1205	0.258163	0.00168034				
		34.93	0.1816	0.256874	0.00251847				
		35.24	0.3160	0.254685	0.00434130				
		36.74	0.1355	0.244624	0.00178042				
		37.00	0.1442	0.242964	0.00188045				
		38.76	0.1056	0.232328	0.00130988				
		38.94	0.1814	0.231295	0.00223887				
		41.20	0.1797	0.219115	0.00208604				
		41.48	0.0007	0.217700	8.066E-060				
		41.83	0.0890	0.215959	0.00101615				

		41.97	0.0763	0.215271	0.00086797				
		43.43	0.0790	0.208367	0.00086554				
		44.17	0.1580	0.205046	0.00169908				
		45.50	0.1185	0.199357	0.00123303				
		46.48	0.1185	0.195380	0.00120405				
		48.41	0.1891	0.188032	0.00183551				
		48.57	0.1016	0.187450	0.00098252				
		52.46	0.2183	0.174430	0.00193321				
		53.00	0.1555	0.172779	0.00136085				
		54.93	0.0785	0.167157	0.00065896				
		55.63	0.1127	0.165218	0.00093209				
		55.79	0.1643	0.164782	0.00135426				
		57.11	0.1857	0.161283	0.00148892				
		59.61	0.1962	0.155103	0.00149450				
		59.78	0.2028	0.154702	0.00153948				
		66.50	0.1665	0.140607	0.00110809				
		66.68	0.1340	0.140271	0.00088875				
		66.88	0.1205	0.139900	0.00079618				
		67.25	0.2156	0.139220	0.00141458				
		72.36	0.1090	0.130596	0.00065030				
		72.61	0.1813	0.130207	0.00107672				
		73.42	0.0790	0.128970	0.00046229				
		75.67	0.1309	0.125685	0.00073541				
		75.87	0.1115	0.125403	0.00062416				
		76.58	0.2078	0.124417	0.00114849				
		79.57	0.1625	0.120476	0.00085147				
		11.05	0.4549	0.800723	0.02051987				
		11.24	0.5510	0.787230	0.02443202				
		12.30	0.4040	0.719616	0.01635964				
		15.74	0.1009	0.563032	0.00318503				
		16.65	0.0903	0.532459	0.00269260				
		16.92	0.0731	0.524023	0.00214444				
		17.90	0.1154	0.495548	0.00319720				
		18.87	0.2302	0.470288	0.00604439				
		19.01	0.1896	0.466856	0.00494102				
		19.48	0.1889	0.455697	0.00480177				
		19.71	0.2090	0.450431	0.00524949				
		20.11	0.1019	0.441561	0.00250750				
		20.35	0.1411	0.436408	0.00343031				
		20.57	0.0719	0.431790	0.00172888				
		21.10	0.1444	0.421062	0.00338304				
		21.38	0.0233	0.415610	0.00053856				
		21.64	0.2765	0.410675	0.00631251				
		21.89	0.2765	0.406041	0.00623866				
		22.21	0.2765	0.400263	0.00614653				
		22.51	0.2765	0.394996	0.00606251				
		23.22	0.1703	0.383076	0.00361677				
		24.26	0.1556	0.366885	0.00315887				
		24.49	0.1993	0.363491	0.00400687				
		25.08	0.0012	0.355072	2.354E-050				
		25.66	0.1182	0.347177	0.00226457				
		25.89	0.0735	0.344144	0.00139523				
17	Monomer cocrystal (5-7)	26.74	0.1713	0.333395	0.00314472	0.977034	1.047564	8.0	NA
		26.89	0.1212	0.331569	0.00221211				
		27.16	0.1011	0.328334	0.00182621				
		28.04	0.2146	0.318226	0.00374999				
		28.35	0.1079	0.314817	0.00186401				
		28.80	0.1581	0.309999	0.00268675				
		30.70	0.2011	0.291233	0.00319651				
		30.97	0.1690	0.288755	0.00266169				
		31.51	0.4081	0.283929	0.00631168				
		32.18	0.2765	0.278169	0.00418261				
		32.70	0.2765	0.273863	0.00411244				
		33.14	0.1451	0.270327	0.00212782				
		33.55	0.1130	0.267117	0.00163566				
		34.21	0.1308	0.262113	0.00185459				
		34.47	0.0718	0.260195	0.00100988				
		34.98	0.2107	0.256518	0.00291759				
		36.83	0.2274	0.244047	0.00298012				
		37.47	0.0012	0.240024	1.5438E-05				
		38.18	0.0856	0.235722	0.00107921				
		38.38	0.2990	0.234540	0.00374850				
		39.62	0.3254	0.227481	0.00394156				
		40.08	0.2765	0.224975	0.00330753				
		40.64	0.1717	0.222004	0.00202313				
		40.95	0.2025	0.220395	0.00236637				
		43.22	0.2765	0.209331	0.00304561				
		43.46	0.2179	0.208230	0.00238554				
		44.22	0.2120	0.204826	0.00227692				
		45.77	0.1975	0.198244	0.00204155				

46.64	0.5530	0.194747	0.00559735
47.02	0.5530	0.193261	0.00554668
48.69	0.1767	0.187016	0.00170400
49.67	0.2469	0.183554	0.00232777
49.89	0.1630	0.182796	0.00152905
50.15	0.0932	0.181909	0.00086912
50.60	0.3935	0.180396	0.00363227
52.09	0.1266	0.175581	0.00113033
52.40	0.2156	0.174615	0.00191182
52.73	0.5530	0.173600	0.00486826
53.18	0.1024	0.172237	0.00089264
53.36	0.1230	0.171698	0.00106802
54.69	0.1831	0.167833	0.00154491
55.52	0.1084	0.165519	0.00089861
56.27	0.5530	0.163490	0.00451236
56.56	0.1954	0.162720	0.00158476
56.77	0.3663	0.162168	0.00295782
57.38	0.1653	0.160588	0.00131795
57.56	0.1758	0.160129	0.00139645
58.27	0.2892	0.158346	0.00226388
58.82	0.3090	0.156996	0.00239181
60.88	0.0220	0.152168	0.00016335
61.13	0.5361	0.151605	0.00396085
61.49	0.1819	0.150804	0.00133434
61.69	0.1246	0.150363	0.00091039
61.88	0.2404	0.149947	0.00174988
63.32	0.2582	0.146879	0.00182699
63.51	0.1550	0.146486	0.00109270
63.70	0.1969	0.146095	0.00138295
64.35	0.1396	0.144775	0.00096820
65.45	0.2786	0.142606	0.00189171
65.64	0.1230	0.142239	0.00083214
65.83	0.2882	0.141874	0.00194270
66.45	0.1021	0.140700	0.00068014
66.95	0.0851	0.139771	0.00056153
67.21	0.0378	0.139293	0.00024820
67.37	0.5530	0.139001	0.00362007
70.11	0.3121	0.134225	0.00194087
70.64	0.1672	0.133347	0.00102961
70.85	0.2021	0.133003	0.00123971
71.49	0.1445	0.131969	0.00087598
71.69	0.1636	0.131650	0.00098813
72.05	0.0632	0.131081	0.00037921
73.16	0.2119	0.129364	0.00124587
74.14	0.1144	0.127895	0.00066073
74.38	0.5475	0.127541	0.00314843
75.17	0.1031	0.126396	0.00058447
76.55	0.0666	0.124458	0.00036829
76.89	0.4941	0.123992	0.00271571

^a The peak position (2θ) and full-width-of-half-maximum (FWHM) are generated from PXRD spectra and Match! software. ^b The d_{hkl} spacing values are calculated from equation (3). ^c The microstrain (ϵ) values are calculated from equation (4). ^d The crystallite sizes are calculated from equations (1) and (2) and the intercept values from Fig. S7. ^e The dislocation densities are calculated from equation (5). ^f R_p is the R factor in Rietveld refinement, showing the discrepancy index between the experimental and calculated spectra. Normally, R_p less than 10% indicates a good fit. ^g Match ratio (%) = (the number of peaks of the polymer identically matched with those of the monomer (red)) / Σ {(the number of peaks of the polymer identically matched with those of the monomer) + (the number of shifted peaks in the polymer (blue)) + (the number of new peaks appeared in the polymer (green, if applicable)) + (the number of peaks present in the monomer but disappeared in the polymer (green, if applicable))} \times 100%. The matching ratio was calculated in pairs (entries 10 vs 11 and entries 13 vs 14).

7. I_{405} and I_{488} values

Table S3 I_{405} and I_{488} values determined with CM showing XB-Driven AIEE (Step 1) and XB-Driven CEE via SPP (Steps 2 and 3) (Figs. S18 and S19)

Entry	Mode ^a	Sample ^b	I_{405} (a.u.) ^c	I_{488} (a.u.) ^c	I_{488} increasing ratio (times, ×)	Entry	Mode ^a	Sample ^b	I_{405} (a.u.) ^c	I_{488} (a.u.) ^c	I_{488} increasing ratio (times, ×)
1	Pure linker	1	NA ^d	1.17		21 ^e	Pure linker	1	NA ^d	1.17	
2	4-comp monomer solid	1-6	NA ^d	4.16	×3.6 from 1	22	4-comp monomer solid	1-7	NA ^d	1.71	×1.5 from 1
3	3-comp polymer sheet	P(1-6)	NA ^d	22.3	×5.4 from 1-6	23	3-comp polymer sheet	P(1-7)	NA ^d	17.5	×10 from 1-7
4	4-comp polymer sheet	P(1-6)	NA ^d	129	×31 from 1-6	24	4-comp polymer sheet	P(1-7)	NA ^d	40.5	×24 from 1-7
5	Pure linker	2	79.3	7.10		25 ^e	Pure linker	2	79.3	7.10	
6	4-comp monomer solid	2-6	214	19.8	×2.8 from 2	26	4-comp monomer solid	2-7	183	10.0	×1.4 from 2
7	3-comp polymer sheet	P(2-6)	NA ^d	82.7	×4.2 from 2-6	27	3-comp polymer sheet	P(2-7)	NA ^d	45.1	×4.5 from 2-7
8	4-comp polymer sheet	P(2-6)	NA ^d	87.3	×4.4 from 2-6	28	4-comp polymer sheet	P(2-7)	NA ^d	200	×20 from 2-7
9	Pure linker	3	223	6.14		29 ^e	Pure linker	3	223	6.14	
10	4-comp monomer solid	3-6	244	9.44	×1.5 from 3	30	4-comp monomer solid	3-7	NA ^d	14.5	×2.4 from 3
11	3-comp polymer sheet	P(3-6)	NA ^d	212	×22 from 3-6	31	3-comp polymer sheet	P(3-7)	NA ^d	120	×8.3 from 3-7
12	4-comp polymer sheet	P(3-6)	NA ^d	221	×23 from 3-6	32	4-comp polymer sheet	P(3-7)	NA ^d	130	×8.9 from 3-7
13	Pure linker	4	41.4	0.40		33 ^e	Pure linker	4	41.4	0.40	
14	4-comp monomer solid	4-6	252	16.3	×41 from 4	34	4-comp monomer solid	4-7	NA ^d	8.61	×22 from 4
15	3-comp polymer sheet	P(4-6)	NA ^d	56.7	×3.5 from 4-6	35	3-comp polymer sheet	P(4-7)	NA ^d	57.7	×6.7 from 4-7
16	4-comp polymer sheet	P(4-6)	NA ^d	61.3	×3.8 from 4-6	36	4-comp polymer sheet	P(4-7)	NA ^d	184	×21 from 4-7
17	Pure L	5	1.57	0.059		37 ^e	Pure L	5	1.57	0.059	
18	4-comp monomer solid	5-6	160	8.99	×150 from 5	38	4-comp monomer solid	5-7	24.9	0.310	×5.3 from 5
19	3-comp polymer sheet	P(5-6)	NA ^d	12.3	×1.4 from 5-6	39	3-comp polymer sheet	P(5-7)	NA ^d	44.0	×140 from 5-7
20	4-comp polymer sheet	P(5-6)	NA ^d	16.3	×1.8 from 5-6	40	4-comp polymer sheet	P(5-7)	NA ^d	52.5	×170 from 5-7

^a 4-comp monomer solid = four-component monomer solid (step 1), 3-comp polymer sheet = three-component polymer sheet (covalently non-crosslinked system) (step 2), and 4-comp polymer sheet = four-component polymer sheet (covalently crosslinked system) (step 3). ^b P denotes polymer. ^c I_{405} and I_{488} values were determined from CM emission intensities at 498 nm and 564 nm, respectively, at a constant area (10 $\mu\text{m} \times 10 \mu\text{m}$) for all entries. ^d Not analyzable (> 255 a.u.) due to the detection limit of instrument ($\lambda_{\text{ex}} = 405 \text{ nm}$). ^e Entry 21 = entry 1, entry 25 = entry 5, entry 29 = entry 9, entry 33 = entry 13, and entry 37 = entry 17.

Table S4 I_{405} and I_{488} values of linker **5** in the pure and polymer-embedded forms determined with PL spectroscopy (Fig. 3)

Entry	Sample	I_{405} (a.u.) ^a	I_{488} (a.u.) ^a	I_{405} increasing ratio (times, ×)	I_{488} increasing ratio (times, ×)
1	Pure linker 5	358	0.152		
2	Linker 5 embedded in P4VP by casting	1720	86.6	×5 from 5	×570 from 5
3	Linker 5 embedded in PMMA by casting	415	18.3	×1.2 from 5	×120 from 5
4	Linker 5 embedded in P4VP by SPP (3-component polymer sheet P(5·6))	3220	90.9	×9 from 5	×600 from 5

^a I_{405} and I_{488} values were determined from PL spectra area integrated at 503–635 nm and 420–585 nm, respectively.

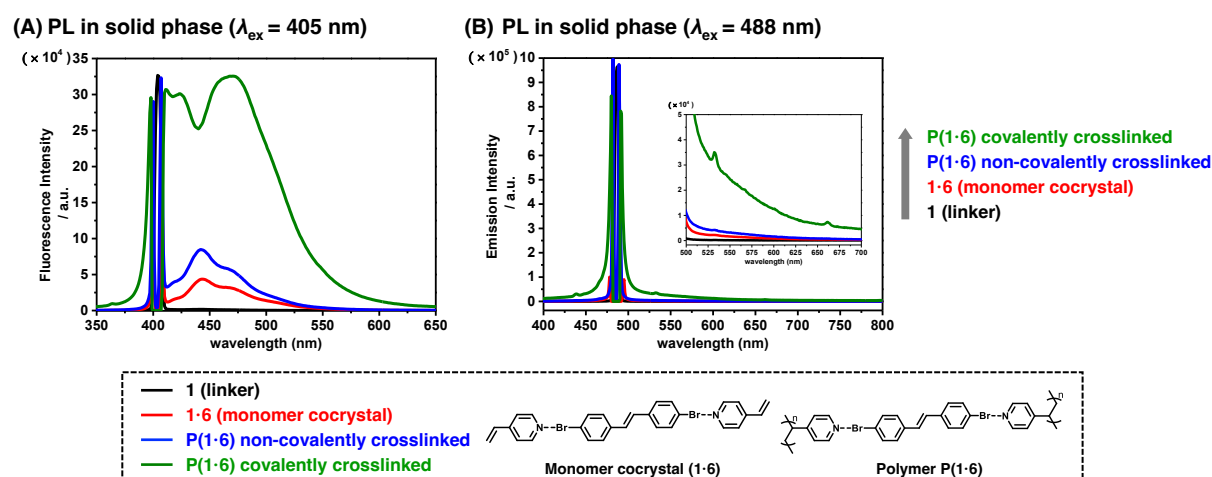


Fig. S9. PL spectra with (A) $\lambda_{\text{ex}} = 405$ nm and (B) $\lambda_{\text{ex}} = 488$ nm for linker **1** (black solid lines), 4-component monomer cocrystal solid (**1·6**) (red solid lines), 3-component non-covalently crosslinked polymer **P(1·6)** (blue solid lines), and 4-component covalently crosslinked polymer **P(1·6)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

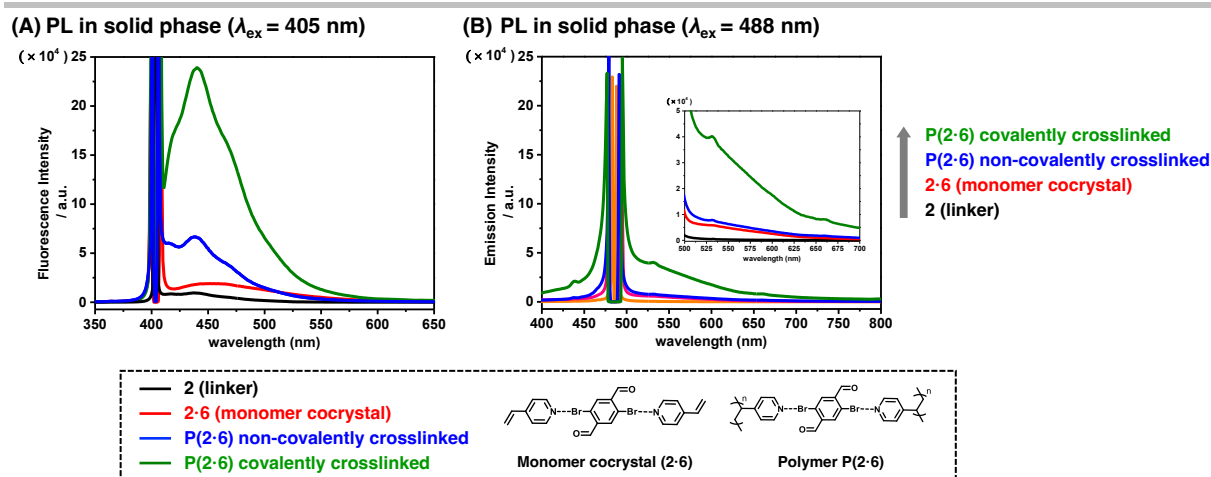


Fig. S10. PL spectra with (A) $\lambda_{\text{ex}} = 405$ nm and (B) $\lambda_{\text{ex}} = 488$ nm for linker **2** (black solid lines), 4-component monomer cocrystal solid (**2·6**) (red solid lines), 3-component non-covalently crosslinked polymer **P(2·6)** (blue solid lines), and 4-component covalently crosslinked polymer **P(2·6)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

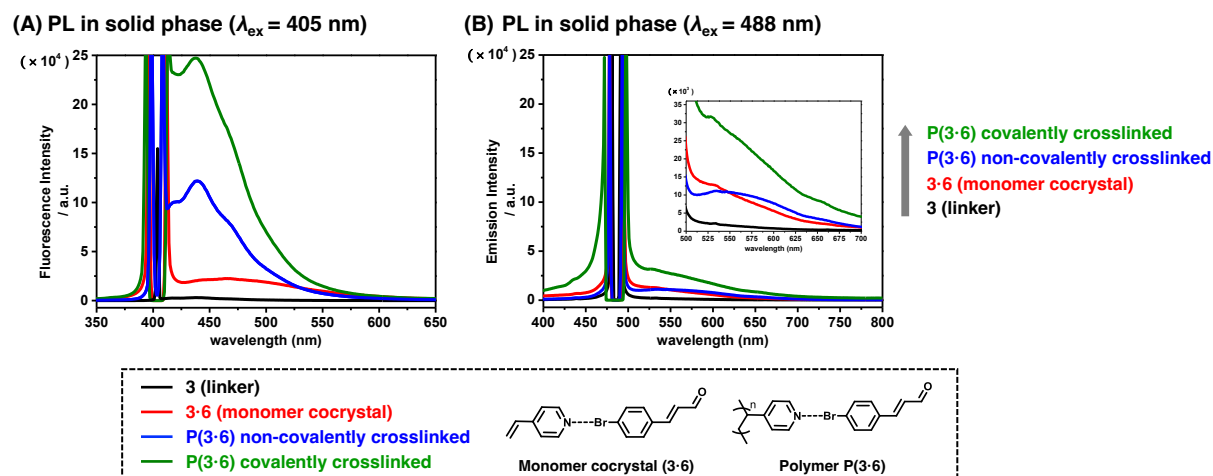


Fig. S11. PL spectra with (A) $\lambda_{\text{ex}} = 405$ nm and (B) $\lambda_{\text{ex}} = 488$ nm for linker **3** (black solid lines), 4-component monomer cocrystal solid (**3·6**) (red solid lines), 3-component non-covalently crosslinked polymer **P(3·6)** (blue solid lines), and 4-component covalently crosslinked polymer **P(3·6)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

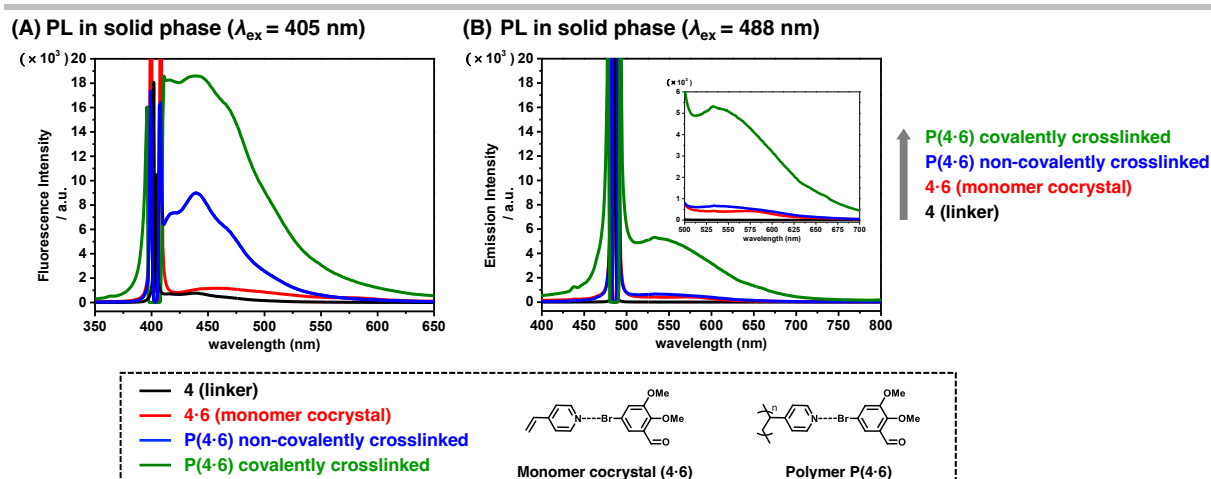


Fig. S12. PL spectra with (A) $\lambda_{ex} = 405$ nm and (B) $\lambda_{ex} = 488$ nm for linker **4** (black solid lines), 4-component monomer cocrystal solid (**4·6**) (red solid lines), 3-component non-covalently crosslinked polymer **P(4·6)** (blue solid lines), and 4-component covalently crosslinked polymer **P(4·6)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

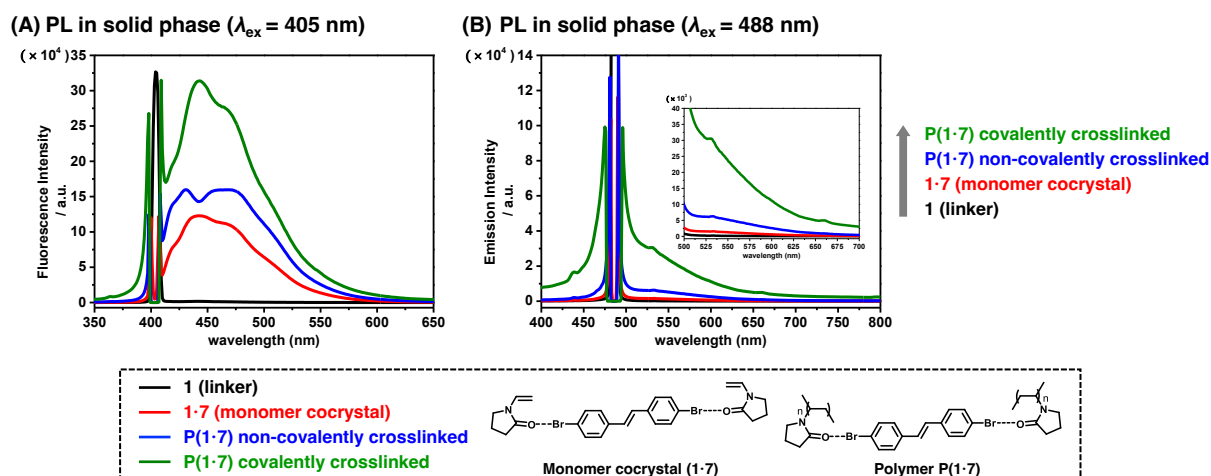


Fig. S13. PL spectra with (A) $\lambda_{ex} = 405$ nm and (B) $\lambda_{ex} = 488$ nm for linker **1** (black solid lines), 4-component monomer cocrystal solid (**1·7**) (red solid lines), 3-component non-covalently crosslinked polymer **P(1·7)** (blue solid lines), and 4-component covalently crosslinked polymer **P(1·7)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

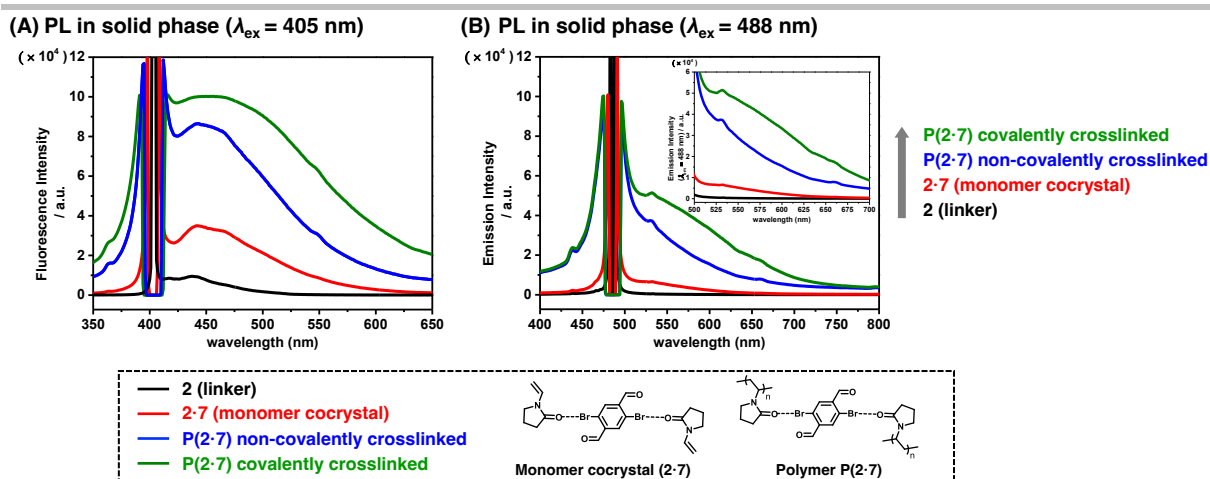


Fig. S14. PL spectra with (A) $\lambda_{\text{ex}} = 405$ nm and (B) $\lambda_{\text{ex}} = 488$ nm for linker **2** (black solid lines), 4-component monomer cocrystal solid (**2·7**) (red solid lines), 3-component non-covalently crosslinked polymer **P(2·7)** (blue solid lines), and 4-component covalently crosslinked polymer **P(2·7)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

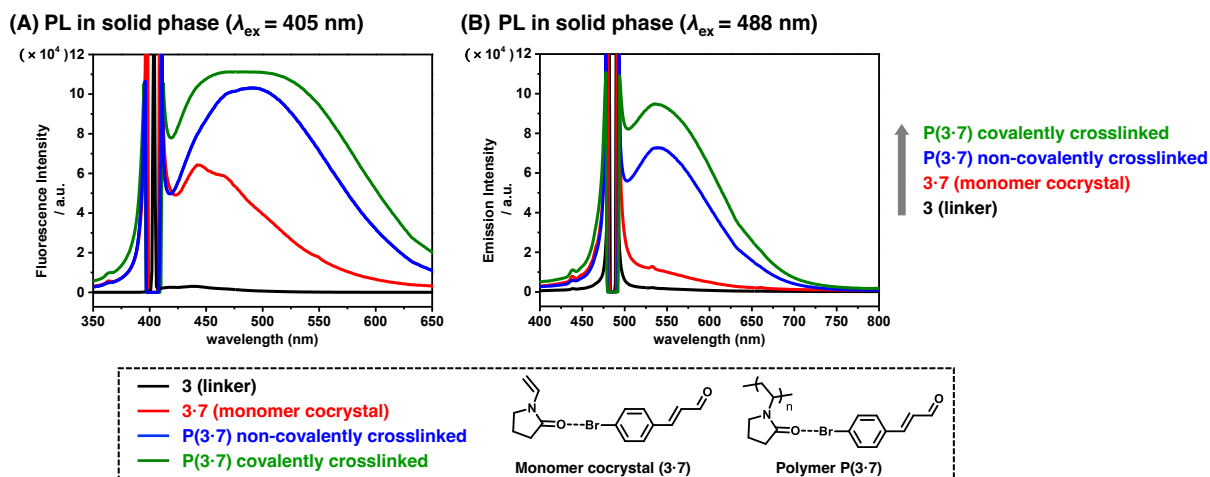


Fig. S15. PL spectra with (A) $\lambda_{\text{ex}} = 405$ nm and (B) $\lambda_{\text{ex}} = 488$ nm for linker **3** (black solid lines), 4-component monomer cocrystal solid (**3·7**) (red solid lines), 3-component non-covalently crosslinked polymer **P(3·7)** (blue solid lines), and 4-component covalently crosslinked polymer **P(3·7)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

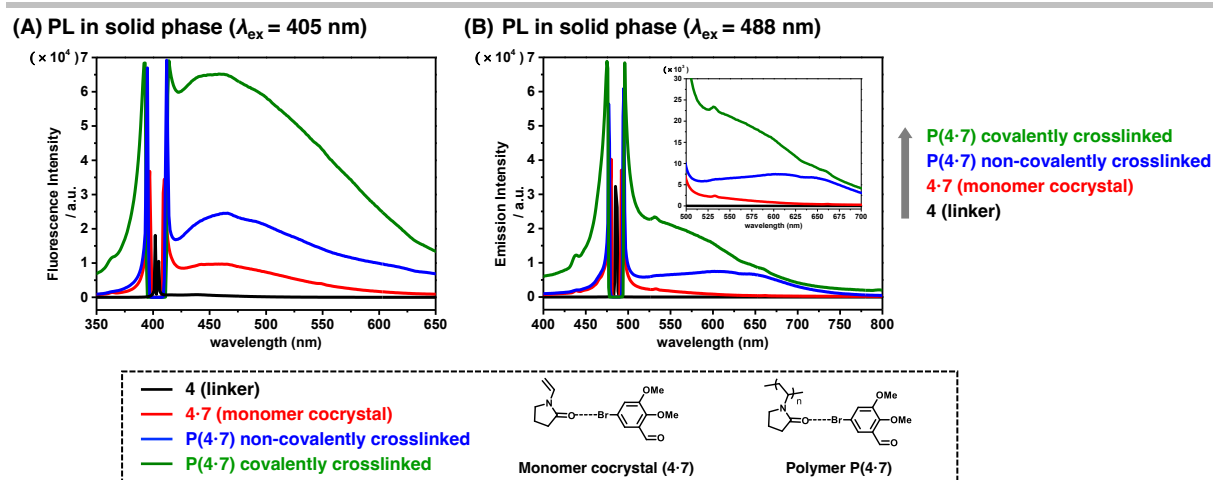


Fig. S16. PL spectra with (A) $\lambda_{ex} = 405$ nm and (B) $\lambda_{ex} = 488$ nm for linker **4** (black solid lines), 4-component monomer cocrystal solid (**4·7**) (red solid lines), 3-component non-covalently crosslinked polymer **P(4·7)** (blue solid lines), and 4-component covalently crosslinked polymer **P(4·7)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

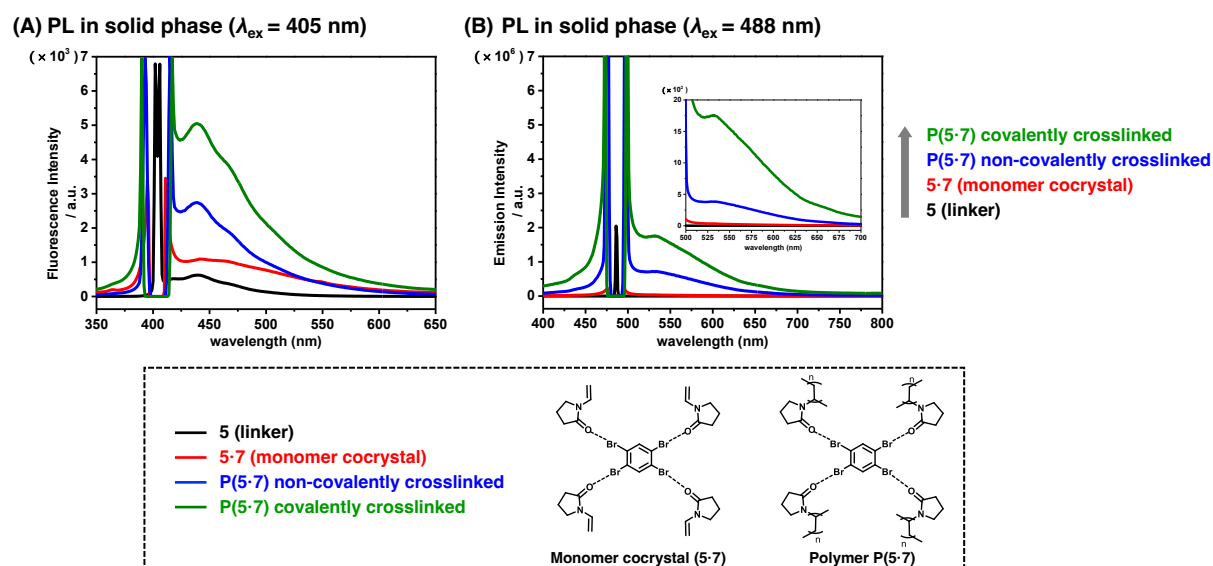


Fig. S17. PL spectra with (A) $\lambda_{ex} = 405$ nm and (B) $\lambda_{ex} = 488$ nm for linker **5** (black solid lines), 4-component monomer cocrystal solid (**5·7**) (red solid lines), 3-component non-covalently crosslinked polymer **P(5·7)** (blue solid lines), and 4-component covalently crosslinked polymer **P(5·7)** (green solid lines). All the sample mass was 0.10 g with a thickness of 1 mm.

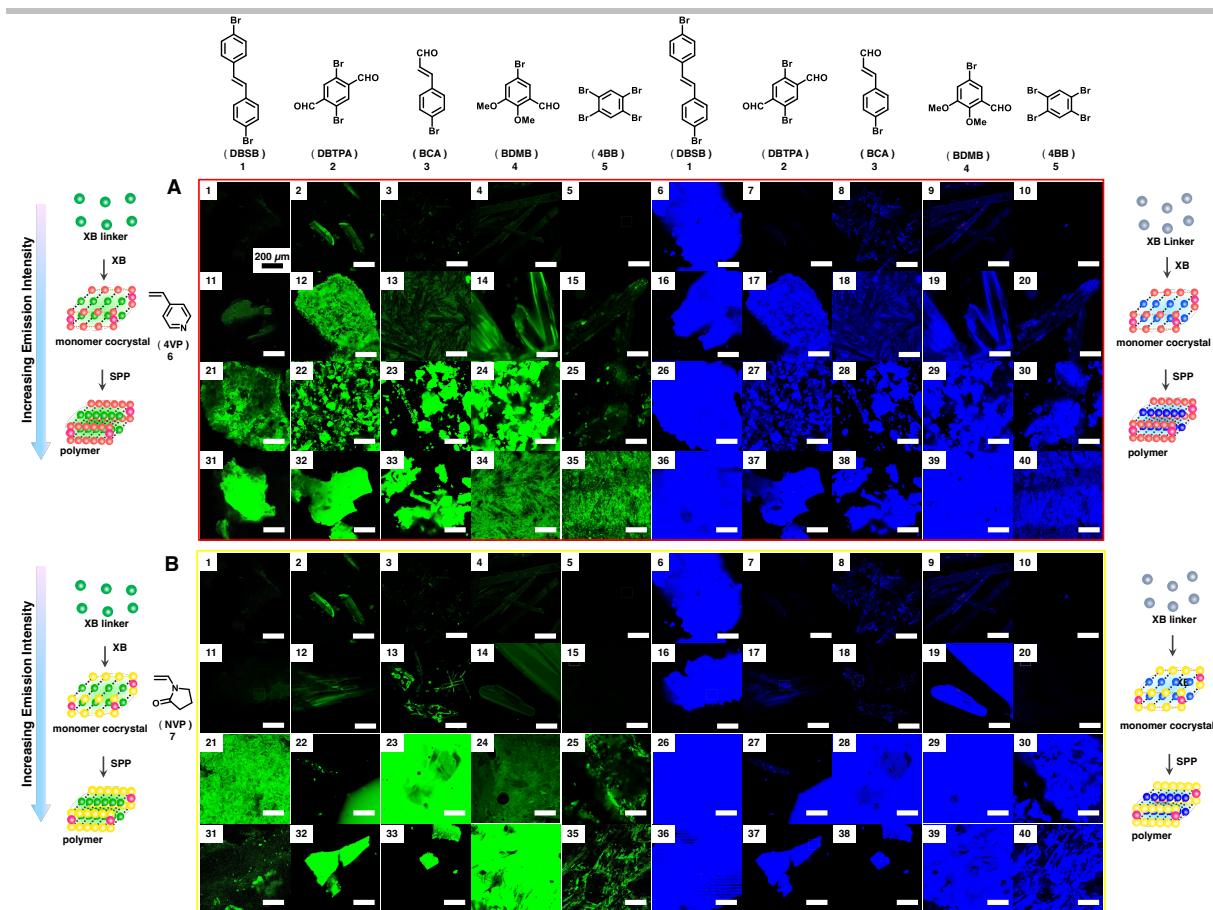


Fig. S18. CM images with $\lambda_{\text{ex}} = 405$ nm and $\lambda_{\text{ex}} = 488$ nm (Scale bar: 200 μm) and I_{405} and I_{488} values of (A) Pure linkers (1–5) (first row, images A1–A10), 4-component monomer cocrystal solids 1·6, 2·6, 3·6, 4·6, and 5·6 (second row, images A11–A20), 3-component non-covalently crosslinked polymers P(1·6), P(2·6), P(3·6), P(4·6), and P(5·6) (third row, images A21–A30), and 4-component covalently crosslinked polymers P(1·6), P(2·6), P(3·6), P(4·6), and P(5·6) (fourth row, images A31–A40). (B) Pure linkers (1–5) (first row, images B1–B10) (same as images A1–A10), 4-component monomer cocrystal solids 1·7, 2·7, 3·7, 4·7, and 5·7 (second row, images B11–B20), 3-component non-covalently crosslinked polymers P(1·7), P(2·7), P(3·7), P(4·7), and P(5·7) (third row, images B21–B30), and 4-component covalently crosslinked polymers P(1·7), P(2·7), P(3·7), P(4·7), and P(5·7) (fourth row, images B31–B40).

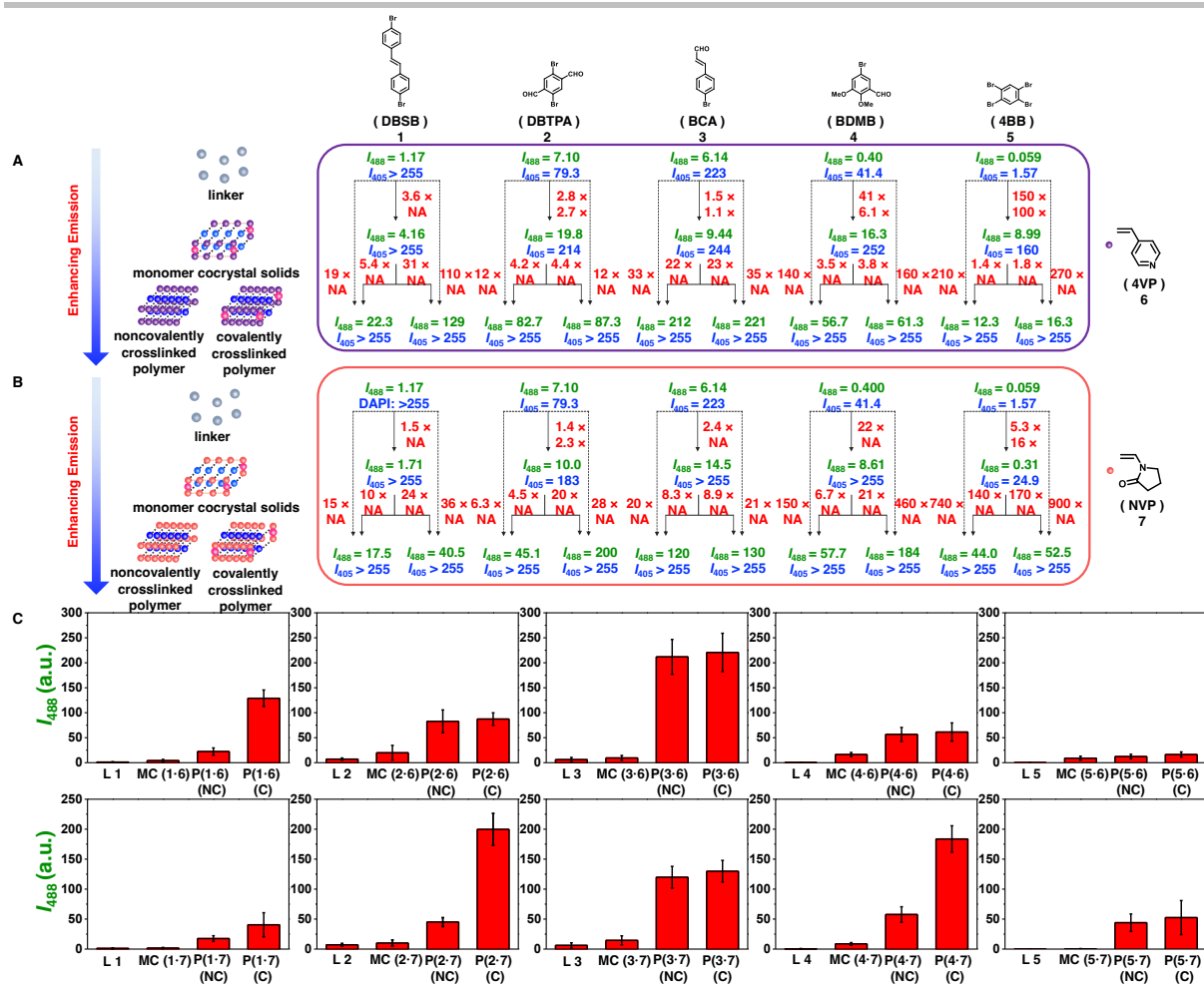


Fig. S19. Summary of Table S3. (A and B) I_{488} (green) and I_{405} (blue) values and emission enhancement (\times , red) of pure linkers (1–5) (first row), 4-component monomer cocrystal solids (second row), and 3-component non-covalently crosslinked polymers (left) and 4-component covalently crosslinked polymers (right) (third row) using (A) monomer 6 and (B) monomer 7. (C) Bar graphs of I_{488} values in (A) and (B) (L = linker, MC = monomer cocrystal solid, NC = non-crosslinked (3-component non-covalently crosslinked) polymer, and C = crosslinked (4-component covalently crosslinked) polymer).

8. Theoretical Calculations

All calculations were executed with Gaussian 09 (Revision A.02) program.² The input molecular structures data in three-dimension (3D with (x,y,z) axes) (cartesian coordinates) were obtained with Chem 3D (version) software. The B3LYP method with the 6-31G(d,p) basis set was utilized for structural optimization and vibrational frequency calculations. For polymer **P(5·6)** (Fig. 4E and S32), due to a large number of atoms, a model polymer **P(5·6)** structure was constructed at a linker/monomer ratio of $\frac{1}{2}$, where three linker molecules are linked to two short polymer chains with six monomer units.

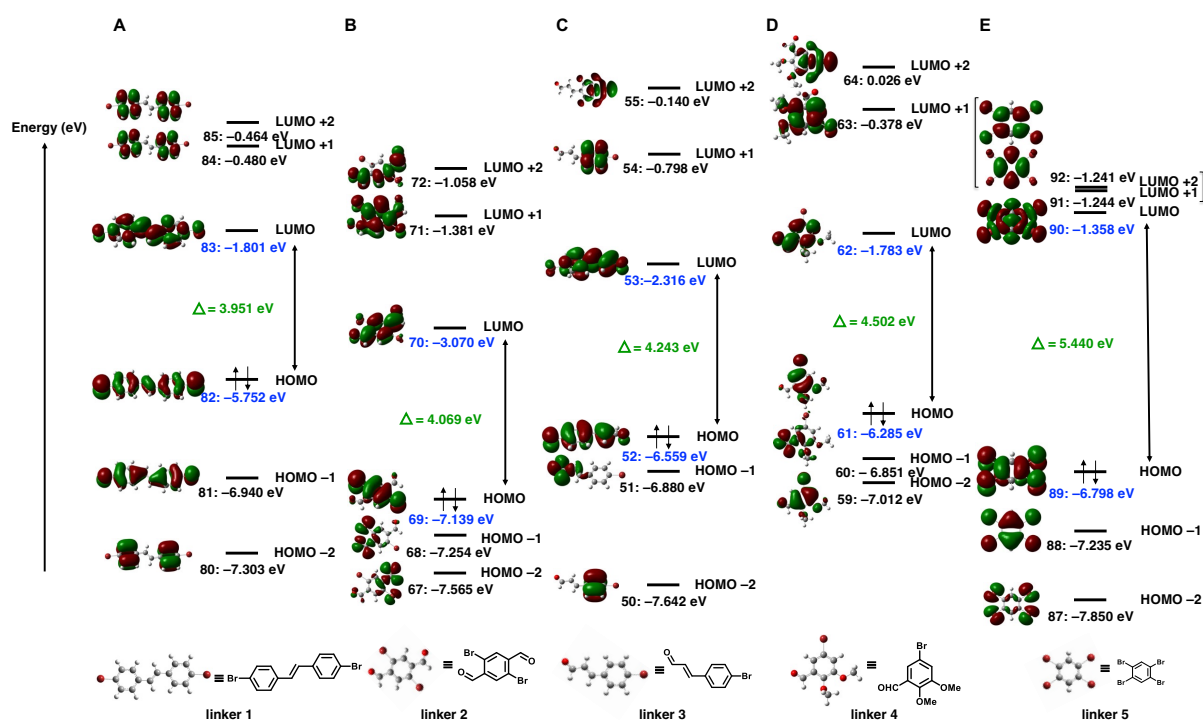


Fig. S20. DFT calculations of HOMO and LUMO for five pure linkers **1–5**, (A) pure linker **1**, (B) pure linker **2**, (C) pure linker **3**, (D) pure linker **4**, and (E) pure linker **5** using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green.

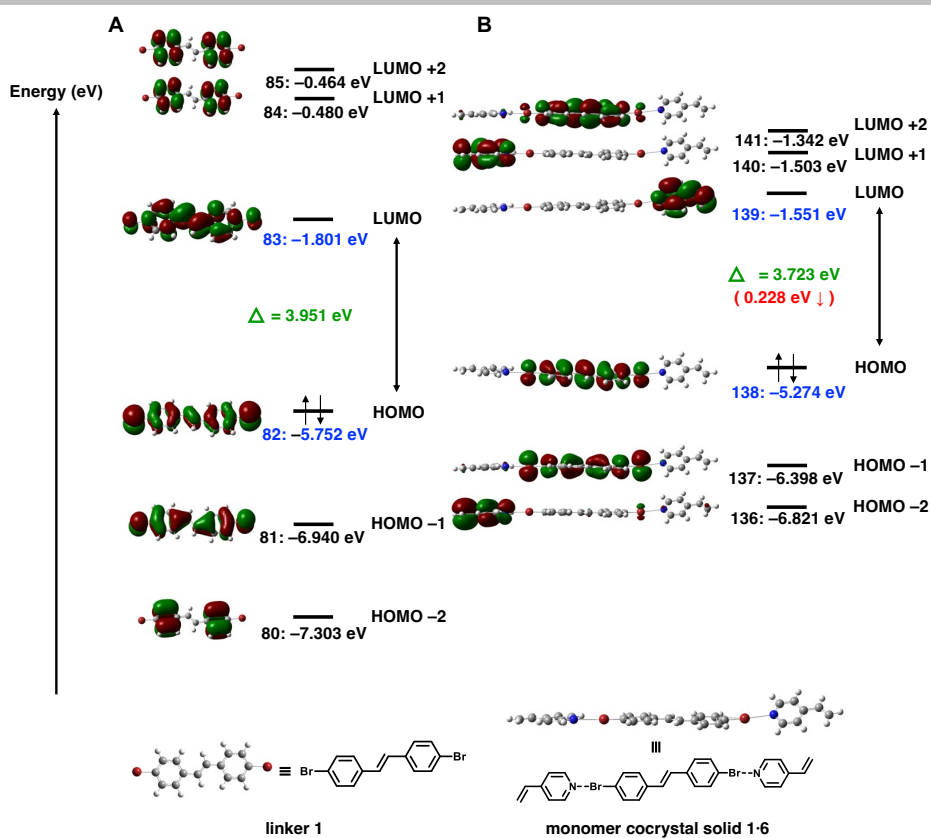


Fig. S21. DFT calculations of HOMO and LUMO for (A) pure linker **1** and (B) monomer cocrystal solid **1·6** at the linker/monomer ratio of $\frac{1}{2}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

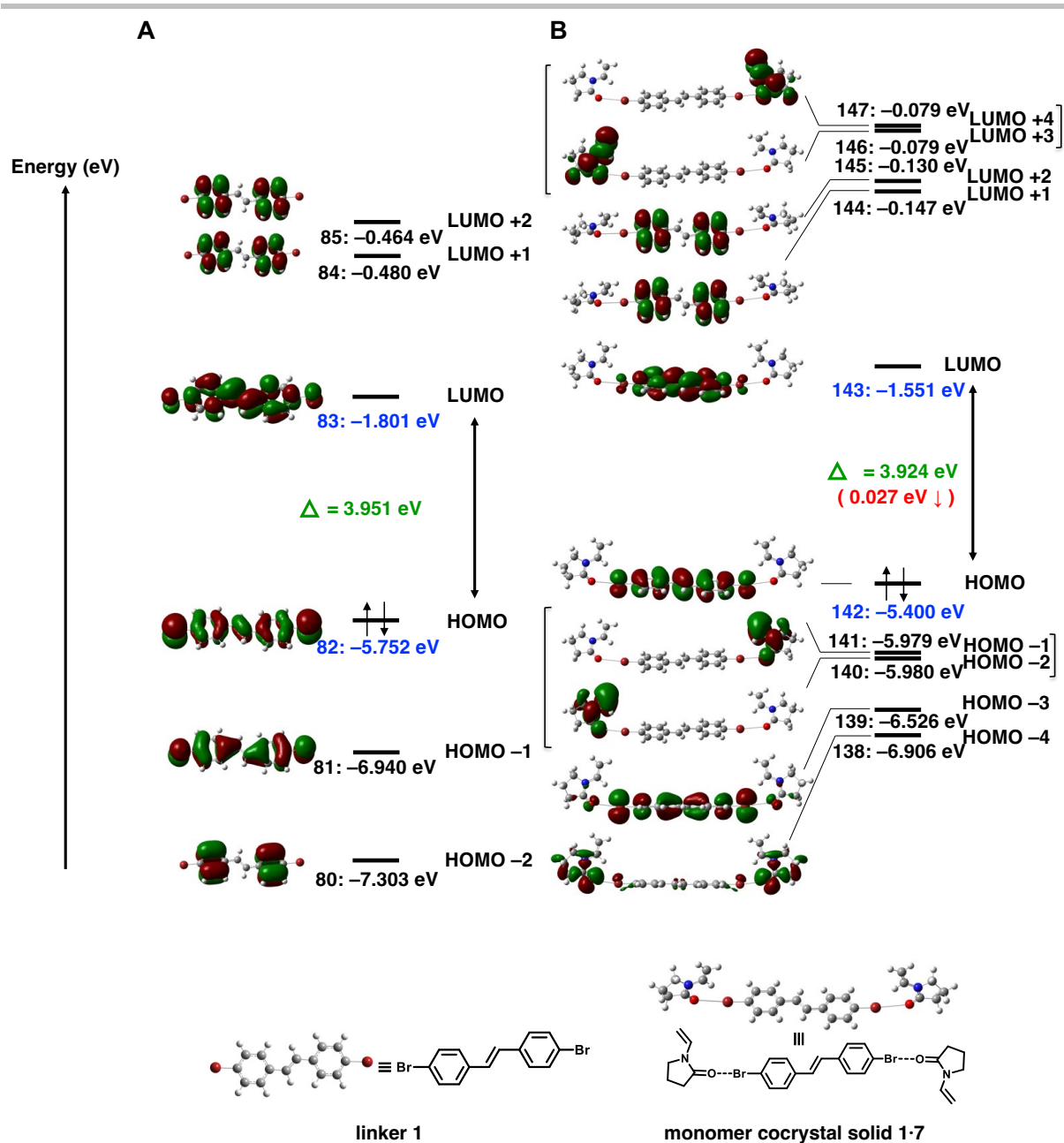


Fig. S22. DFT calculations of HOMO and LUMO for (A) pure linker 1 and (B) monomer cocrystal solid 1·7 at the linker/monomer ratio of $\frac{1}{2}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

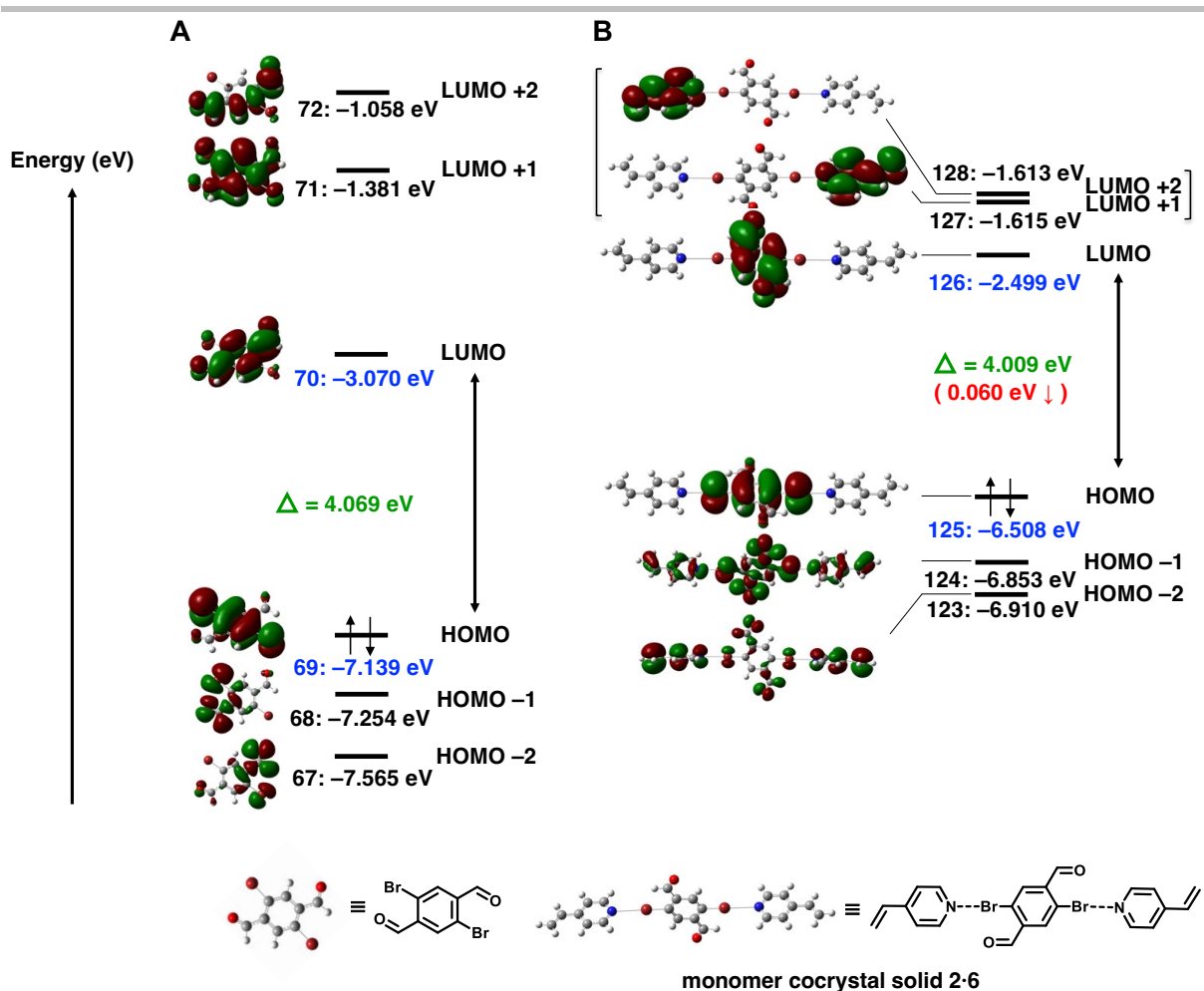


Fig. S23. DFT calculations of HOMO and LUMO for (A) pure linker **2** and (B) monomer cocrystal solid **2·6** at the linker/monomer ratio of $\frac{1}{2}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

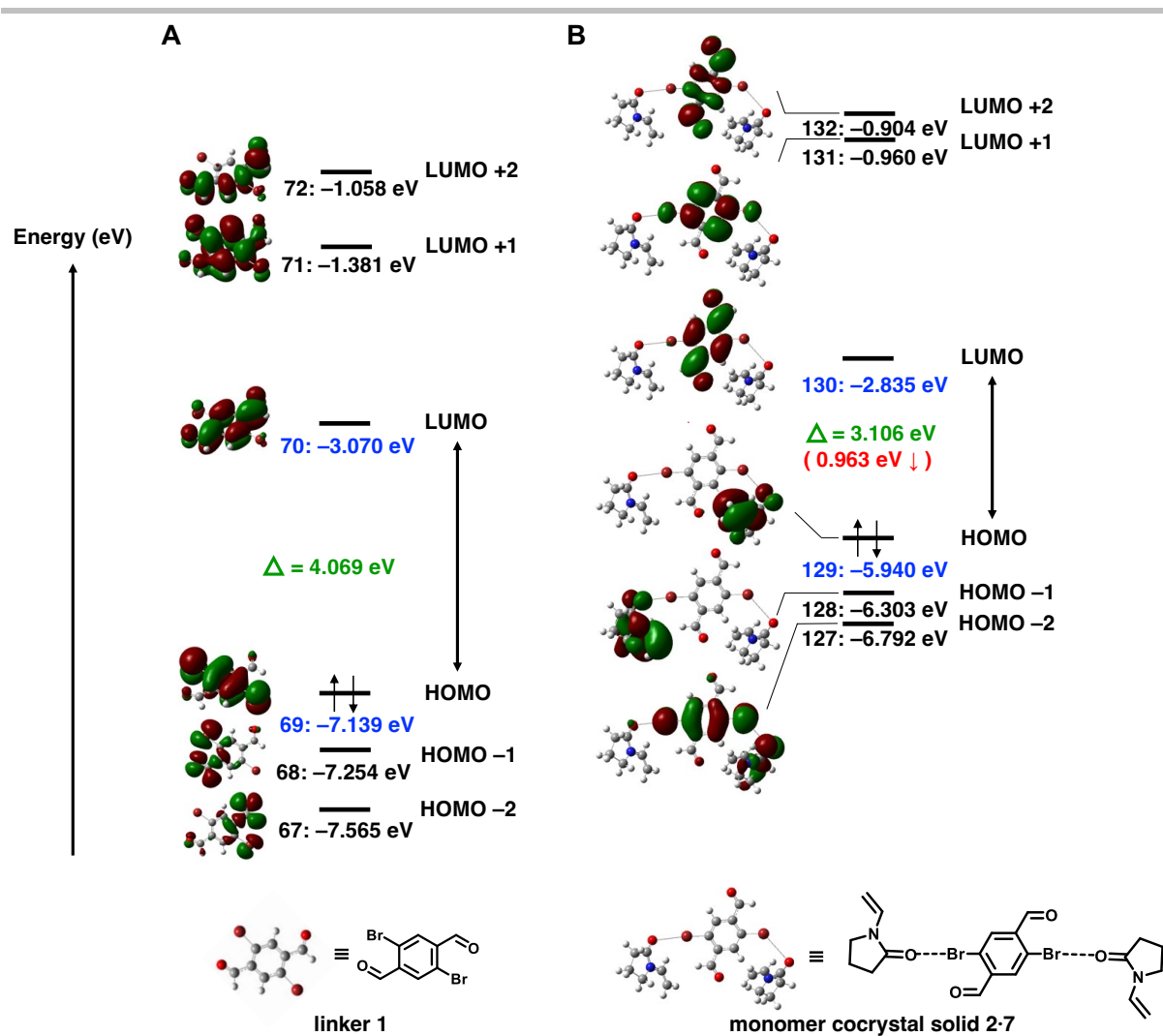


Fig. S24. DFT calculations of HOMO and LUMO for (A) pure linker 2 and (B) monomer cocrystal solid 2·7 at the linker/monomer ratio of $\frac{1}{2}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

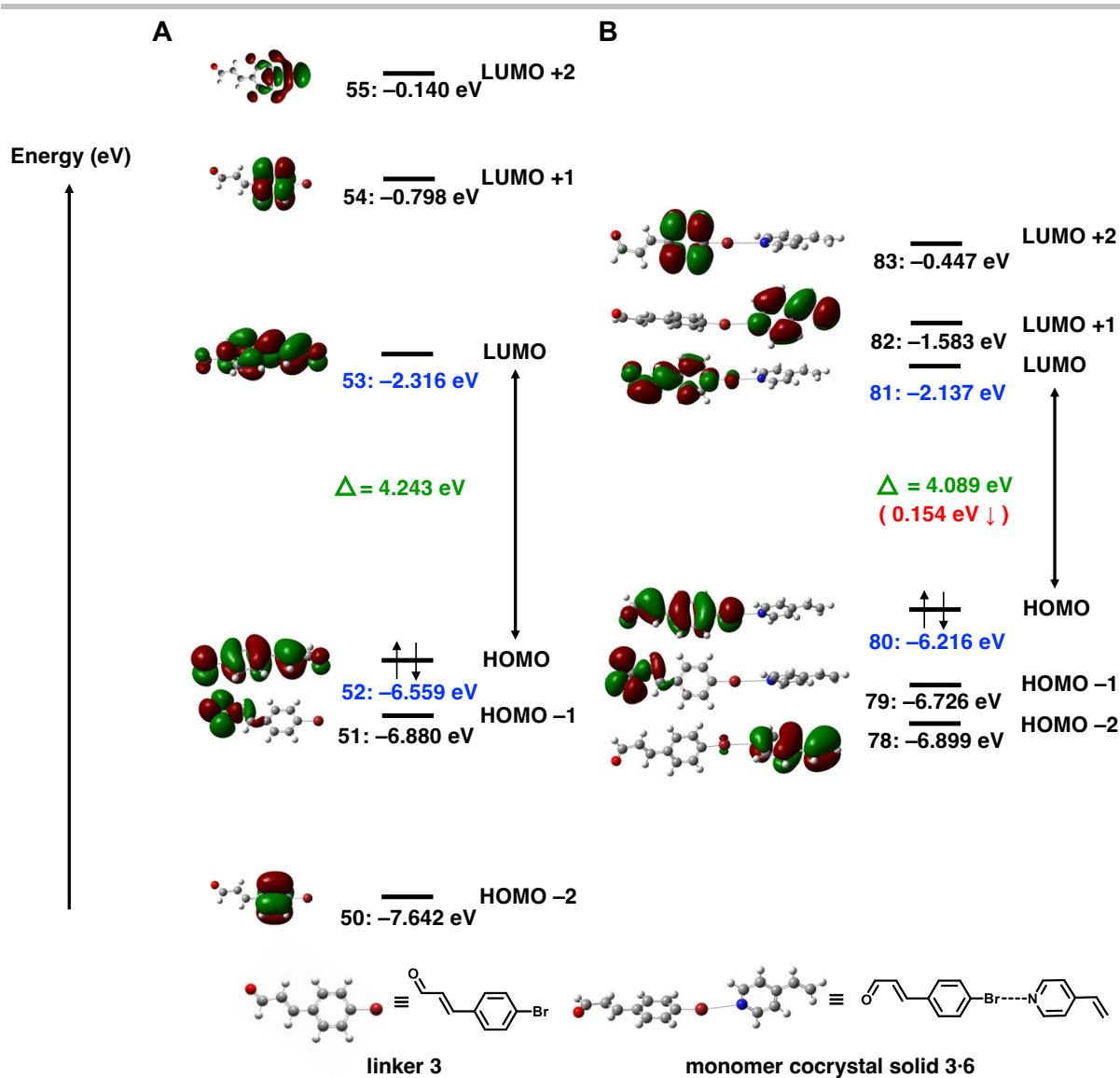


Fig. S25. DFT calculations of HOMO and LUMO for (A) pure linker **3** and (B) monomer cocrystal solid **3·6** at the linker/monomer ratio of 1/1 using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

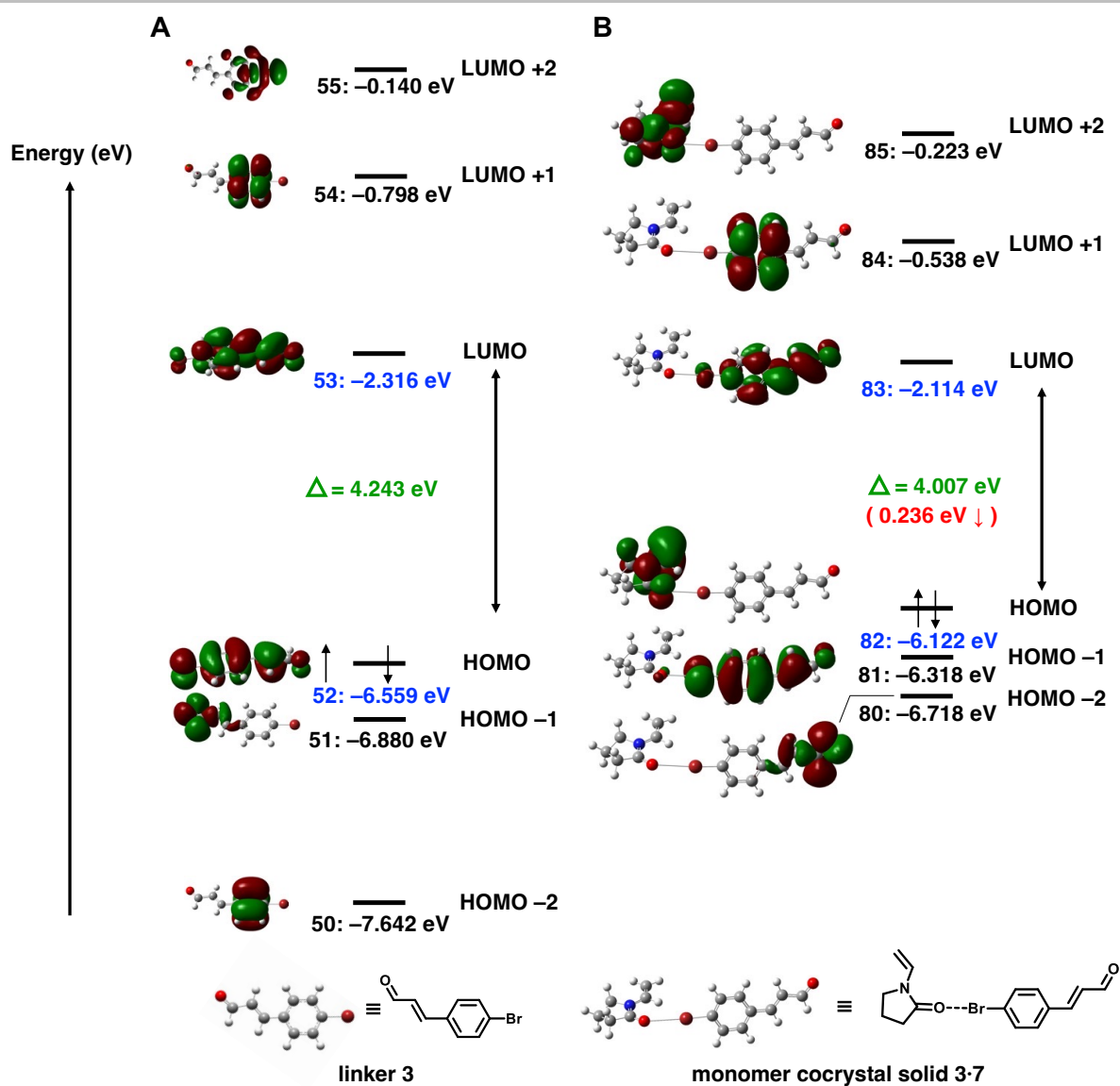


Fig. S26. DFT calculations of HOMO and LUMO for (A) pure linker **3** and (B) monomer cocrystal solid **3·7** at the linker/monomer ratio of 1/1 using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

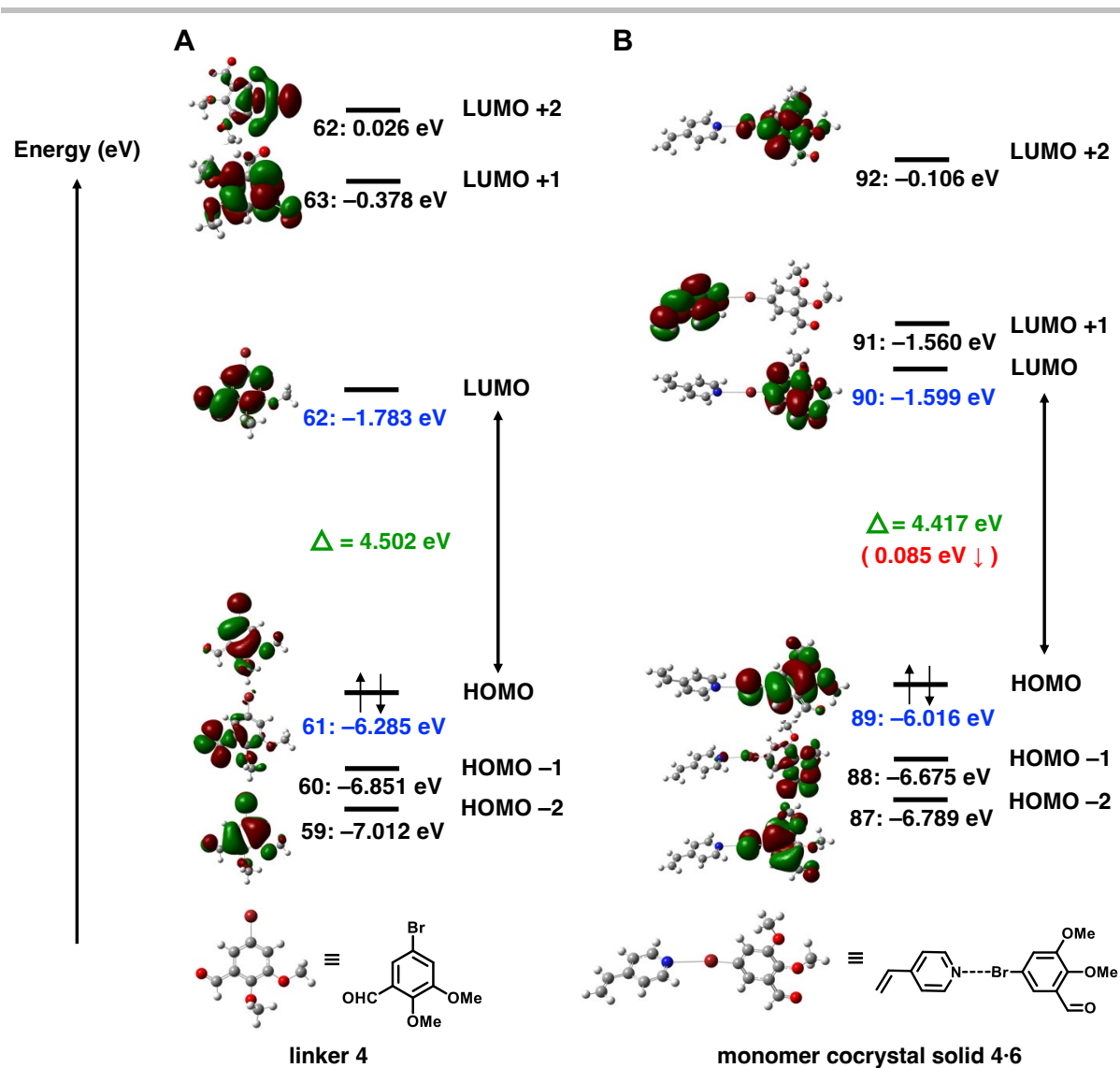


Fig. S27. DFT calculations of HOMO and LUMO for (A) pure linker 4 and (B) monomer cocrystal solid 4·6 at the linker/monomer ratio of 1/1 using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

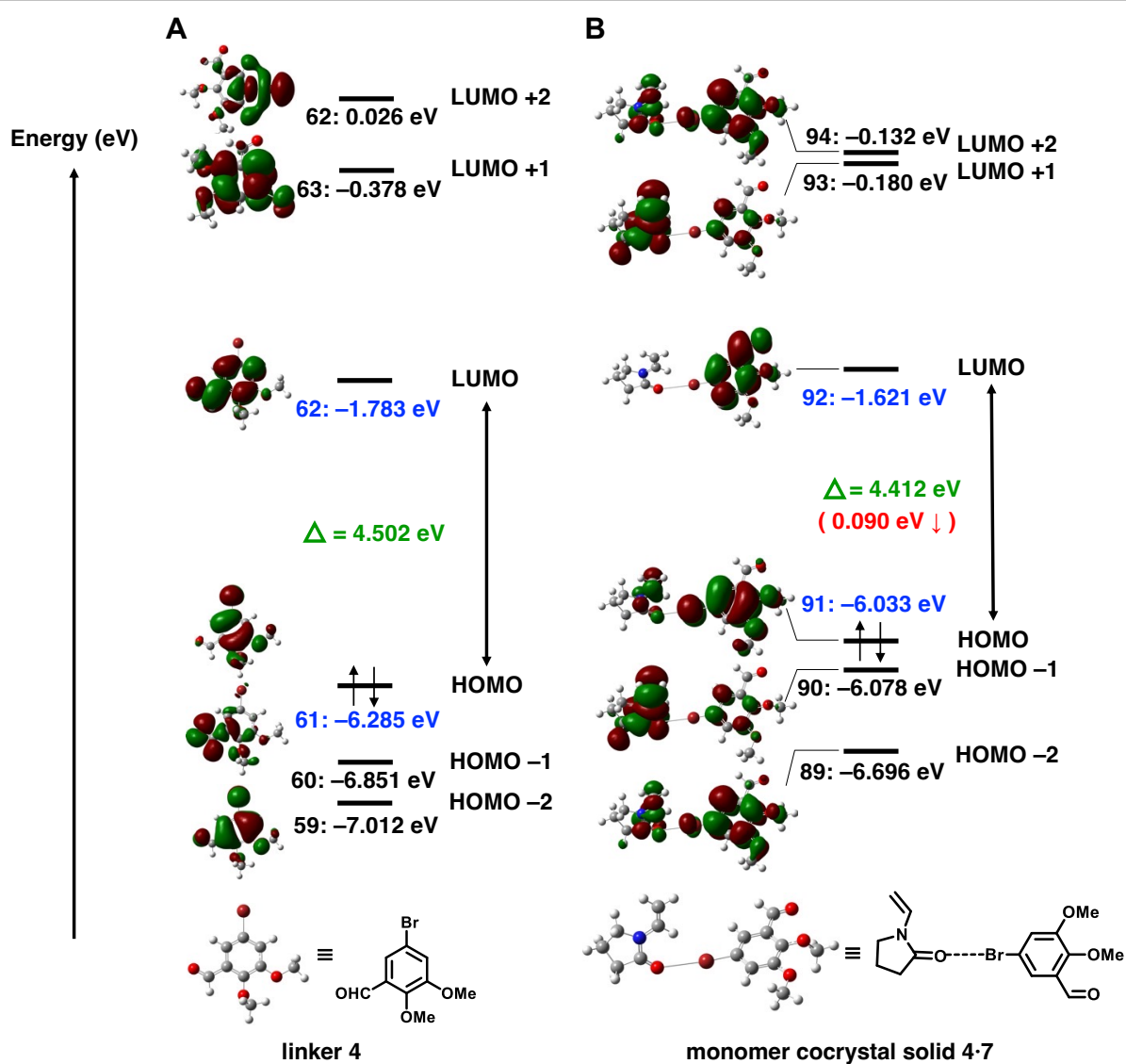


Fig. S28. DFT calculations of HOMO and LUMO for (A) pure linker 4 and (B) monomer cocrystal solid 4·7 at the linker/monomer ratio of 1/1 using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

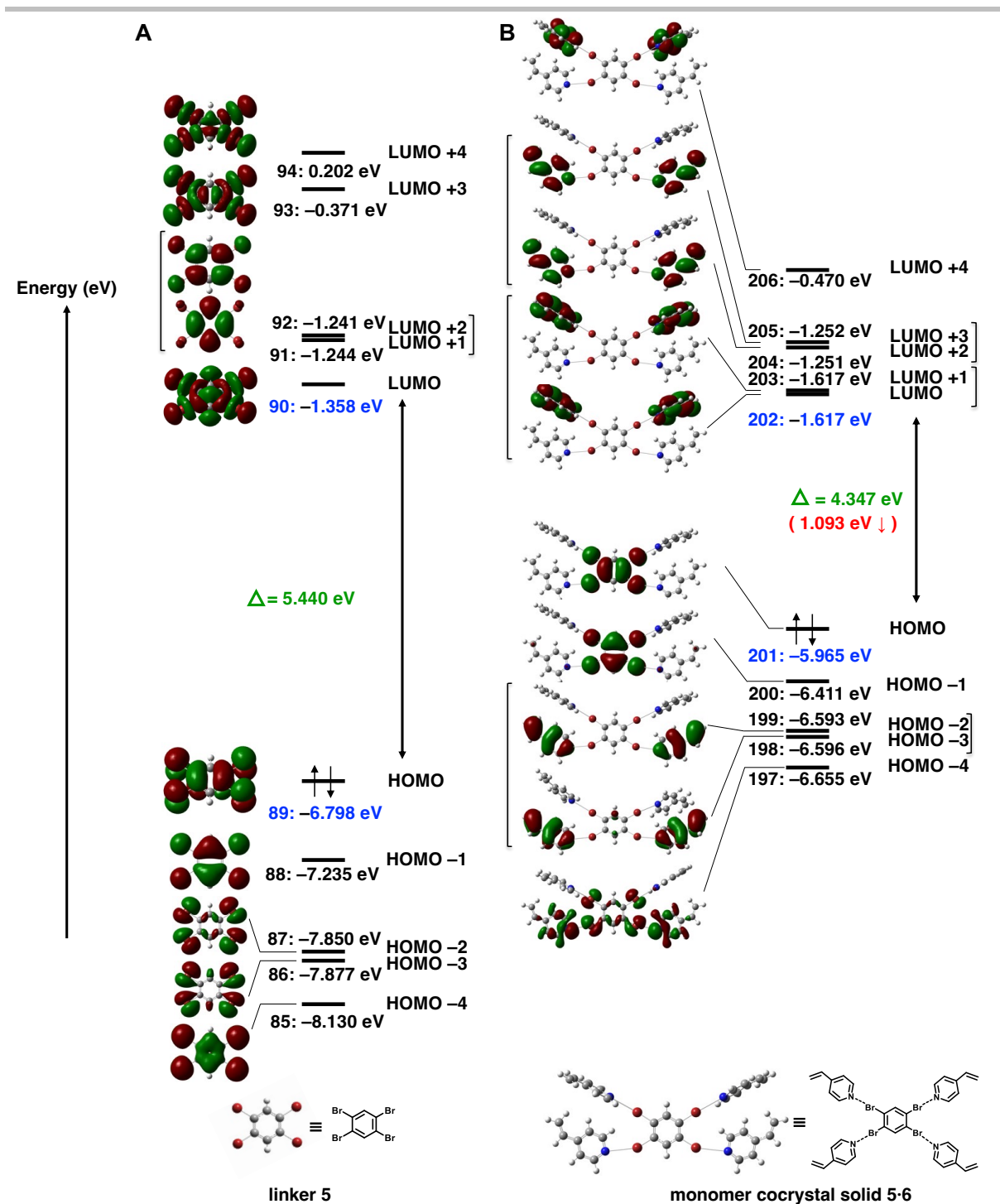


Fig. S29. DFT calculations of HOMO and LUMO for (A) pure linker **5** and (B) monomer cocrystal solid **5·6** at the linker/monomer ratio of $\frac{1}{4}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

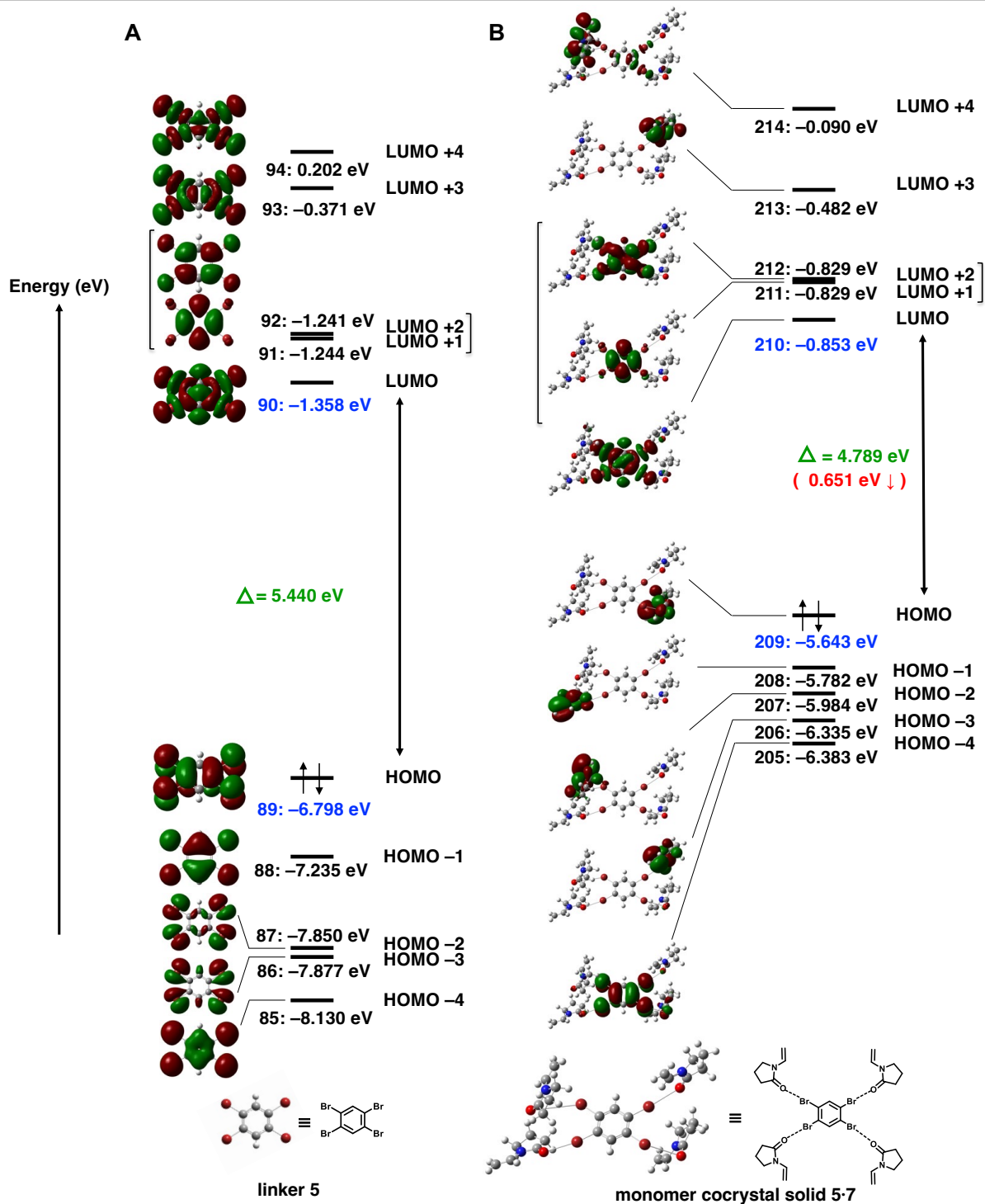


Fig. S30. DFT calculations of HOMO and LUMO for (A) pure linker **5** and (B) monomer cocrystal solid **5·7** at the linker/monomer ratio of $\frac{1}{4}$ using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B) is given in red.

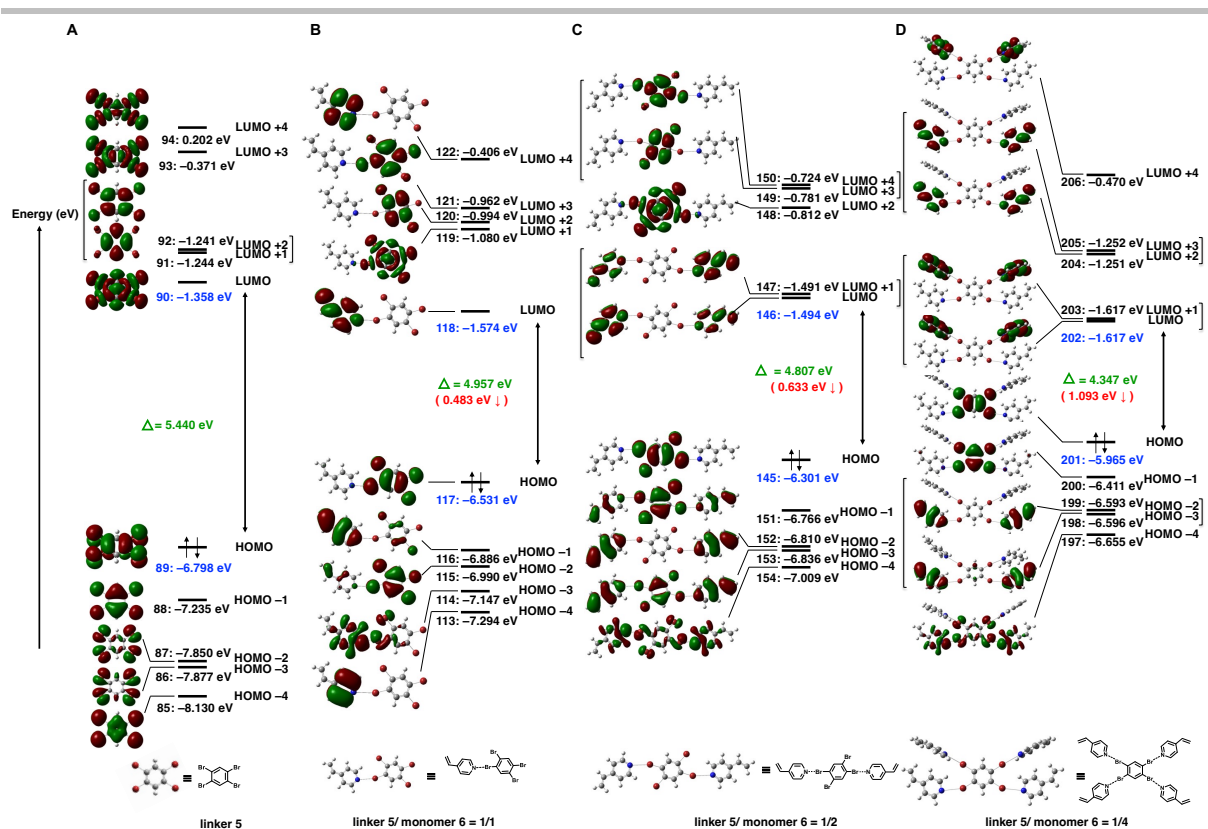


Fig. S31. DFT calculations of HOMO and LUMO for (A) pure linker **5**, and monomer cocrystals **5·6** at the linker/monomer ratios of (B) 1/1, (C) 1/2, and (D) 1/4 using B3LYP/6-31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B-D) is given in red (details of Figs. 4A-4D).

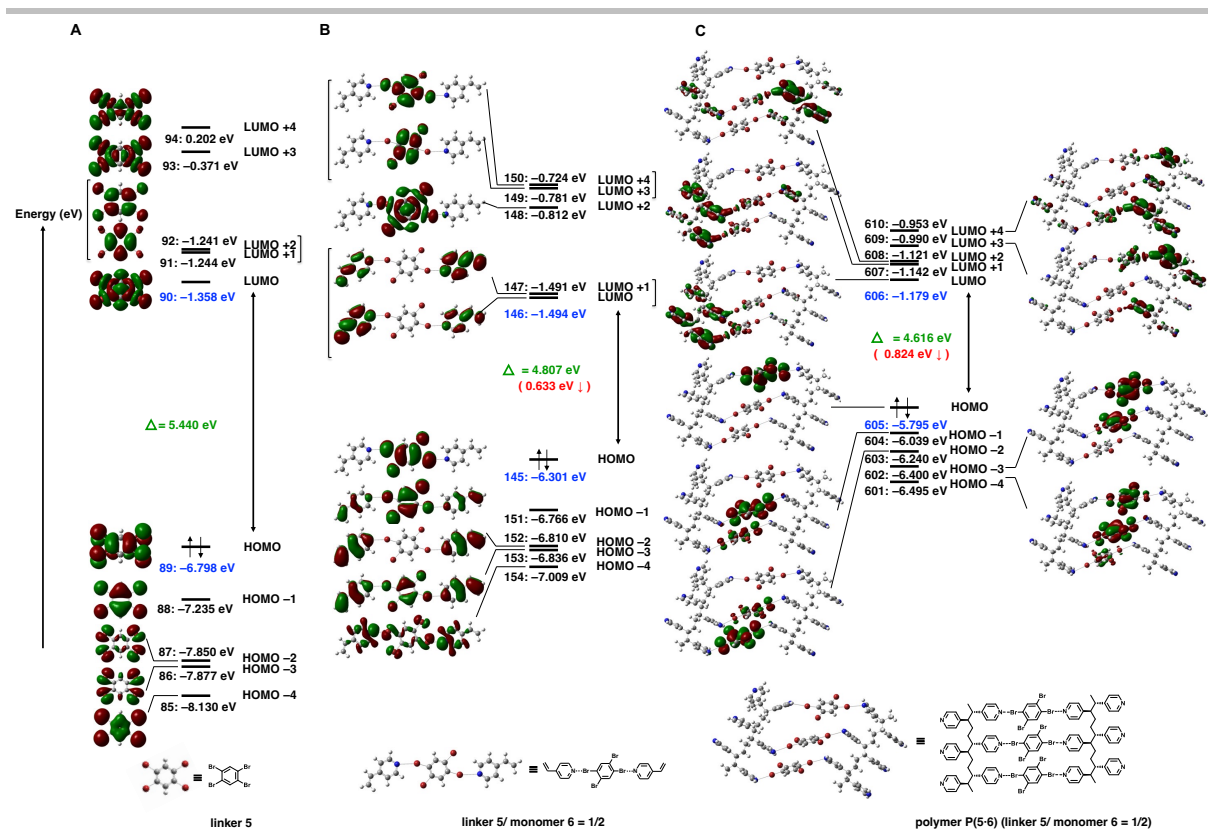


Fig. S32. DFT calculations of HOMO and LUMO for (A) pure linker **5**, (B) monomer cocrystals **5·6** at the linker/monomer ratio of $\frac{1}{2}$, and (C) model polymer **P(5·6)** at the linker/monomer ratio of $\frac{1}{2}$, using B3LYP/6–31G(d,p) level of theory. The HOMO-LUMO gap is given in green. The decrease in the HOMO-LUMO gap from (A) to (B and C) is given in red (details of Figs. 4A, 4C, and 4E).

9. Patterned Emissive Polymer Sheet

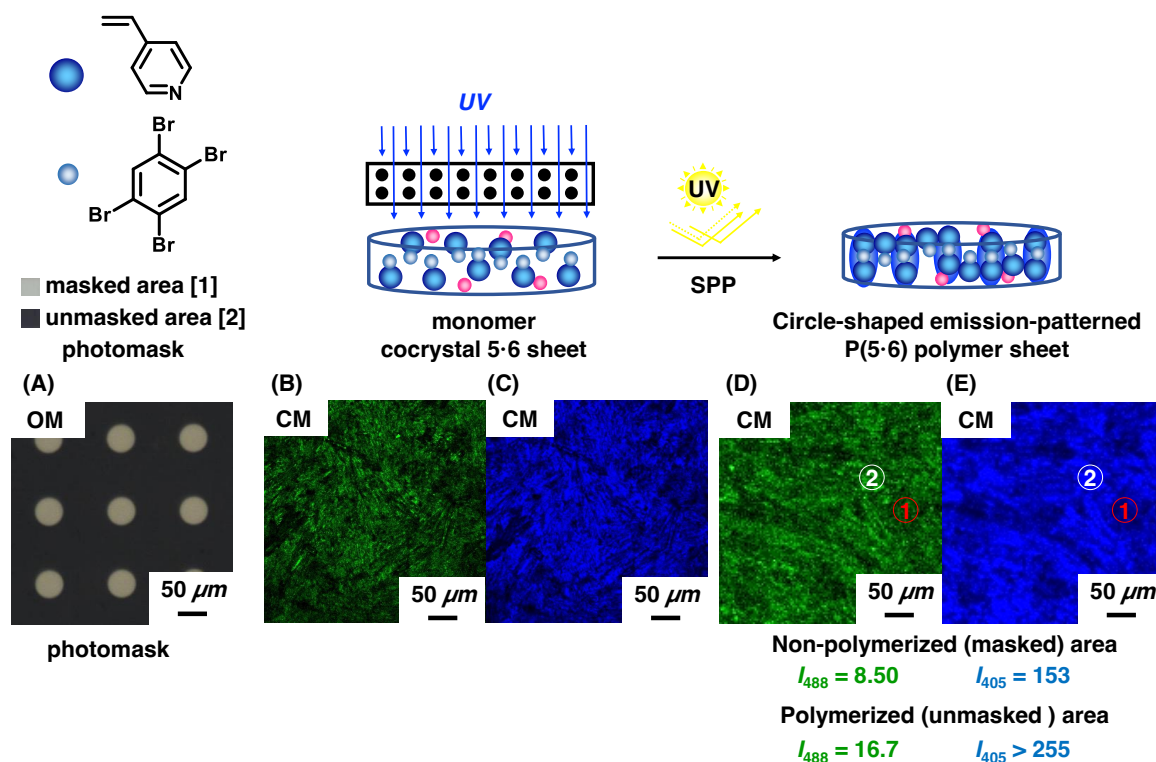


Fig. S33. Schematic illustrations of the preparation of emission-patterned polymer sheet, (A) OM image of photomask circle 50, CM images with (B) $\lambda_{ex} = 488$ nm and (C) $\lambda_{ex} = 405$ nm of monomer cocystal (5·6) (before SPP), CM images with (D) $\lambda_{ex} = 488$ nm and (E) $\lambda_{ex} = 405$ nm of polymer sheet P(5·6) (after SPP).

10. Thermal Stability

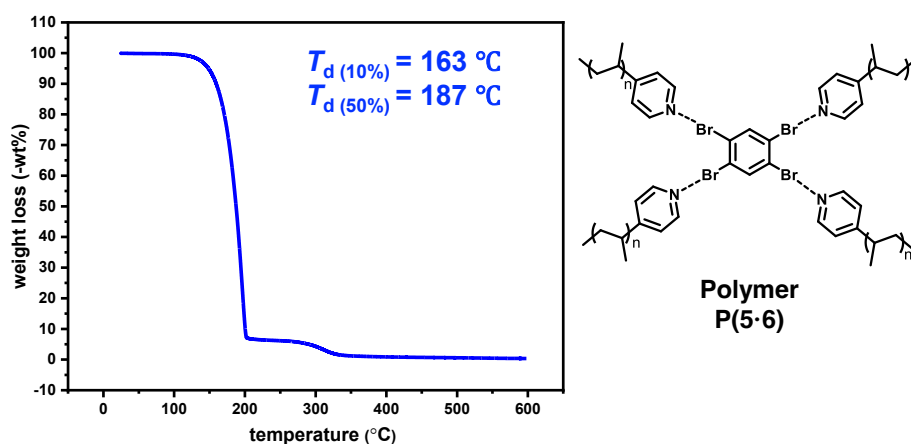


Fig. S34. TGA curve of the 4-component covalently crosslinked polymer sheet P(5·6) ($T_{d(10\%)} = 163$ °C and $T_{d(50\%)} = 187$ °C).

11. Emission of P4VP synthesized via solution phase radical polymerization

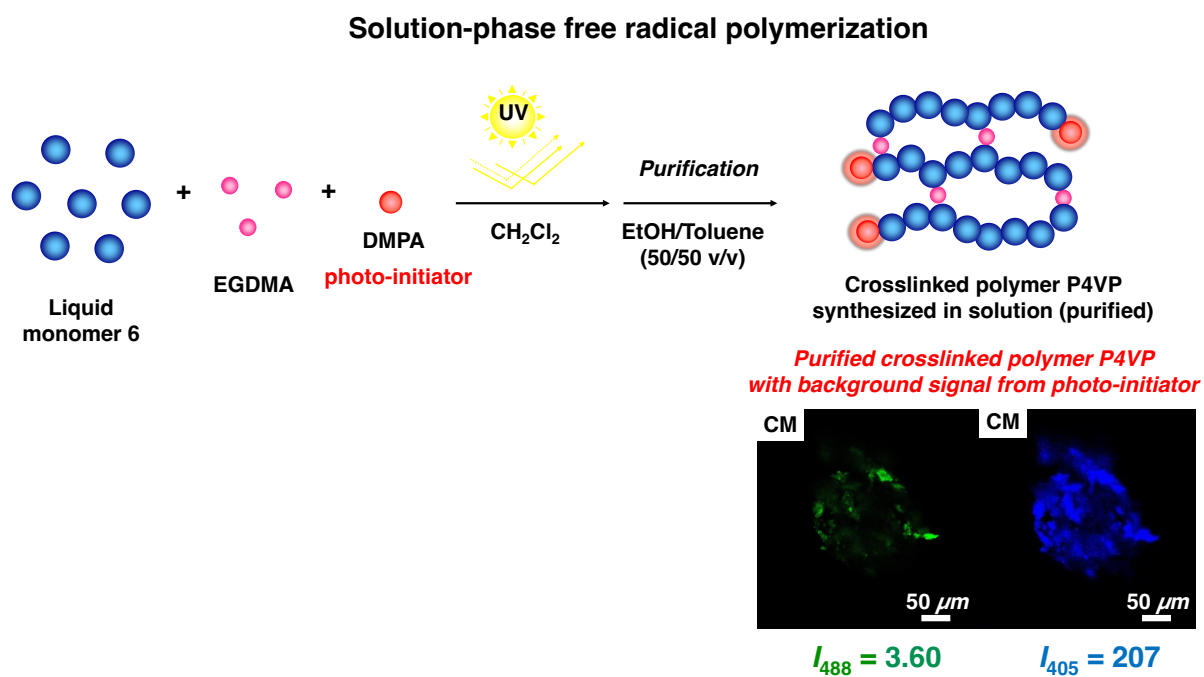


Fig. S35. Schematic illustration of the purified crosslinked polymer P4VP synthesized via solution-phase free radical polymerization of liquid monomer 6, EGDMA, and DMPA (photo-initiator) and CM images of the purified crosslinked polymer P4VP with $\lambda_{\text{ex}} = 488$ nm (left) and $\lambda_{\text{ex}} = 405$ nm (right).

12. Cartesian Coordinates

Atom Coordinates (Angstroms)
X Y Z

XB linker 4 (BDMB)

XB linker 1 (DBSb)

C -1.802099 3.735112 -0.040949
C -1.721630 2.414640 -0.280432
C -0.548295 1.760896 -0.357382
C 0.569874 2.488793 -0.251228
C 0.512810 3.837275 -0.074332
C -0.645794 4.482055 0.039515
C -0.576068 0.416448 -0.420522
C 0.463939 -0.392412 -0.371290
C 0.481648 -1.763005 -0.241725
C 1.701655 -2.383520 -0.184624
C 1.741391 -3.738775 -0.048322
C 0.577873 -4.468624 0.156101
C -0.594146 -3.861977 0.051101
C -0.649670 -2.514752 -0.130138
Br -0.699621 6.349754 0.164494
Br 0.776830 -6.352709 0.188096
H -2.826442 4.147591 0.061638
H -2.670391 1.922072 -0.366785
H 1.616601 2.122120 -0.210237
H 1.526053 4.304540 -0.305688
H -1.587881 -0.100908 -0.504937
H 1.459183 0.090092 -0.308575
H 2.687812 -1.785924 -0.253508
H 2.752128 -4.134657 -0.028836
H -1.527767 -4.424049 0.197401
H -1.656940 -2.054192 -0.239781

XB linker 2 (DBTPA)

C -1.160975 0.712222 -0.041328
C -1.101314 -0.609582 0.051723
C 0.126014 -1.220204 0.022021
C 1.307374 -0.594911 0.007259
C 1.191068 0.765773 -0.056224
C -0.005471 1.432212 -0.069796
Br 2.547601 1.924542 0.036426
C 2.463665 -1.353752 0.025050
C -2.388710 1.330052 -0.095704
Br -2.625700 -1.834213 0.042164
O -2.518099 2.563956 -0.111145
O 3.560051 -0.914703 -0.104386
H 0.145589 -2.371257 -0.053747
H 0.019638 2.551562 -0.087185
H 2.378193 -2.454633 0.071486
H -3.383533 0.726844 -0.185936

XB linker 3 (BCA)

C -4.383913 1.889593 -0.587498
C -4.004489 0.736218 -0.005746
C -4.882298 -0.229304 0.346719
C -6.169925 -0.040865 0.000333
C -6.647801 1.122383 -0.427424
C -5.677516 2.021980 -0.866289
Br -3.210081 3.367142 -0.876992
C -6.984171 -1.076878 0.300351
C -8.288729 -1.183613 0.203631
C -8.936021 -2.298295 0.669835
O -10.123818 -2.554171 0.644023
H -2.952193 0.595461 0.262512
H -4.534319 -1.125079 0.939066
H -7.675484 1.416758 -0.472700
H -5.970913 2.977708 -1.234431
H -6.495483 -1.853732 0.817369
H -8.911959 -0.401083 -0.195418
H -8.197415 -3.042343 1.099776

O 0.699114 -1.906154 0.099625
C 0.628303 -0.471118 0.142164
C 1.786542 0.226671 0.314789
C 1.874369 1.544682 0.239509
C 0.755199 2.203403 0.028503
C -0.452445 1.620411 -0.108723
C -0.534596 0.237946 0.045373
Br 0.824559 4.025759 -0.108421
C 2.978404 -0.382341 0.507374
O -1.782581 -0.387896 -0.179776
O 4.104766 0.099822 0.635578
C -0.357220 -2.711255 -0.437955
C -2.885525 0.358970 -0.617721
H 2.753053 2.108813 0.409169
H -1.358059 2.206937 -0.109019
H 2.970896 -1.430521 0.515394
H -1.215505 -2.724889 0.272781
H -0.456471 -2.400025 -1.512353
H -0.022905 -3.829805 -0.461440
H -3.294678 1.132626 0.083890
H -2.636449 0.877268 -1.555822
H -3.711406 -0.397227 -0.704168

XB linker 5 (4BB)

C 1.080780 0.692801 0.132796
C 1.199529 -0.656870 0.206968
C 0.099212 -1.391775 0.007259
C -1.091756 -0.737341 0.009447
C -1.226708 0.577753 0.115441
C -0.116829 1.284021 0.192887
Br -2.850049 1.728689 -0.060766
Br -2.569209 -1.906064 0.009928
Br 2.569256 1.845459 -0.014187
Br 2.862169 -1.626178 -0.051454
H 0.082621 -2.467331 -0.122824
H -0.173848 2.389135 0.210763

Monomer solid I□6 (DBSb□4VP)

C -4.207508 -2.774238 -2.840501
C -2.925707 -3.024036 -3.235655
C -1.605990 -2.811948 -3.126734
C -1.202284 -2.028732 -2.137902
C -2.333434 -1.488848 -1.671334
C -3.615201 -1.874312 -1.993778
C 0.079711 -1.649963 -1.827279
C 0.605584 -0.809590 -0.840435
C 1.866506 -0.497420 -0.651806
C 2.170358 0.354158 0.329661
C 3.425937 0.736471 0.490880
C 4.440104 0.390062 -0.272142
C 4.194350 -0.419865 -1.309236
C 2.869454 -0.787442 -1.493781
Br 6.324024 0.816371 0.305261
Br -5.854496 -2.146578 -2.002149
C -9.886598 -0.527459 -0.714581
C -8.888672 0.353640 -0.912720
C -7.696701 -0.181520 -1.248228
N -7.437118 -1.464465 -1.388307
C -8.458375 -2.277721 -1.303362
C -9.692465 -1.876751 -0.997828
C -11.093338 -0.010906 -0.409736
C -12.230119 -0.663628 -0.309867
C 9.019357 2.537969 3.533694
C 7.769428 2.382332 3.240390
C 7.394268 1.910361 2.023290
N 7.961050 1.300571 0.874265
C 9.051720 1.759541 1.416932
C 9.733737 2.264166 2.445601
C 9.493299 3.079767 4.681546
C 10.767821 3.337282 5.052596
H -3.148629 -3.787678 -4.024804
H -0.850554 -3.241257 -3.772351
H -2.121480 -0.713790 -0.887993

H	-0.476308	2.107226	-2.016900	H	-2.868301	-1.212322	-2.158839
H	0.741638	3.074068	-1.064283	H	-4.824122	0.117432	-2.517223
H	-2.005847	2.737020	1.431759	H	-5.384712	-0.074636	-0.749064
H	-0.269898	1.208509	2.033549				
H	0.601662	1.417265	0.398183				
H	-8.837195	-2.264179	2.667587				
H	-9.776625	-3.821452	2.529452				
H	-7.992943	-5.105414	3.492824				
H	-7.706584	-3.567858	4.409044				
H	-5.957237	-2.880707	2.853801				
H	-5.767823	-4.693556	2.841225				
H	-6.407656	-4.024456	-0.767991				
H	-4.069058	-4.438772	-0.495728				
H	-4.171034	-4.299067	1.360887				

Monomer solid 3□6 (BCA□4VP)

C	-6.322047	-4.301609	-0.650895
C	-6.808778	-3.663140	0.426935
N	-8.005961	-3.122108	0.468602
C	-8.768673	-3.514080	-0.464702
C	-8.382870	-4.199334	-1.578875
C	-7.105362	-4.541059	-1.710362
C	-6.617998	-5.226205	-2.737462
C	-7.226442	-5.395356	-3.936880
C	-7.167175	0.590310	0.772675
C	-7.264582	1.114092	1.984079
C	-6.836301	2.395989	2.217817
C	-6.342769	3.233295	1.273333
C	-6.260833	2.644154	0.043297
C	-6.653745	1.376050	-0.161322
Br	-7.656800	-1.296021	0.367565
C	-5.906386	4.446804	1.579898
C	-5.325283	5.342076	0.777148
C	-4.864876	6.602283	1.008133
O	-4.861457	7.243085	2.043410
H	-5.243132	-4.684686	-0.674500
H	-6.170608	-3.619304	1.266719
H	-9.872996	-3.402101	-0.235144
H	-9.219207	-4.393056	-2.242439
H	-5.604211	-5.634741	-2.783535
H	-6.673890	-5.877077	-4.754615
H	-8.405609	-5.267916	-4.070586
H	-7.714354	0.494189	2.750880
H	-7.011111	2.817779	3.293752
H	-5.816081	3.257966	-0.726406
H	-6.577525	0.916702	-1.156973
H	-6.030476	4.754388	2.640064
H	-5.156650	5.111955	-0.331909
H	-4.489749	7.224016	0.093741

Monomer solid 3□7 (BCA□NVP)

C	1.484625	-0.202240	-0.540496
C	2.721191	-0.527847	-0.943268
C	3.711944	0.373735	-0.853395
C	3.507039	1.615020	-0.364957
C	2.254595	1.915913	0.032822
C	1.253354	1.024504	-0.051036
Br	0.076752	-1.461503	-0.659688
C	4.549987	2.471100	-0.302913
C	4.545047	3.738916	0.149324
C	5.653481	4.524754	0.171568
O	5.654472	5.665885	0.578096
N	-3.176001	-1.627413	-0.225900
C	-2.150015	-2.325486	0.045876
C	-2.091626	-2.783581	1.497691
C	-3.552007	-2.634728	1.919291
C	-4.026005	-1.508406	0.989837
O	-1.275278	-2.634264	-0.759819
C	-3.548211	-1.062145	-1.302814
C	-4.638838	-0.311815	-1.519686
H	2.937693	-1.530544	-1.349142
H	4.712069	0.056846	-1.198098
H	1.993278	2.903155	0.444170
H	0.243276	1.313436	0.286592
H	5.525818	2.095856	-0.663022
H	3.624420	4.208385	0.530403
H	6.591557	4.060048	-0.212000
H	-1.713832	-3.825746	1.598416
H	-1.439892	-2.086852	2.074833
H	-3.685674	-2.403898	3.000030
H	-4.100180	-3.579261	1.684146
H	-5.113128	-1.650405	0.788367
H	-3.858804	-0.512049	1.464706

Monomer solid 4□6 (BDMB□4VP)

C	-5.451254	-3.500149	2.093772
C	-6.653439	-3.795929	1.618172
N	-6.950738	-3.787644	0.387069
C	-6.026467	-3.878479	-0.491535
C	-4.733831	-3.620492	-0.117744
C	-4.423325	-3.326606	1.162063
C	-3.156061	-3.116728	1.519101
C	-2.782881	-2.773977	2.773835
C	-7.684043	-0.210235	-0.001820
C	-6.874304	0.628202	0.686534
C	-7.038167	2.010303	0.653207
C	-7.982303	2.503998	-0.162739
C	-8.876964	1.732823	-0.805474
C	-8.719268	0.381851	-0.678551
Br	-7.461142	-2.065029	0.073572
C	-6.181472	2.642191	1.442003
O	-6.076318	3.851044	1.598598
O	-8.118304	3.868935	-0.251688
C	-7.187482	4.524269	-1.103743
O	-9.967239	2.236490	-1.557146
C	-11.294457	1.652197	-1.309121
H	-5.231877	-3.549639	3.207716
H	-7.465810	-4.114061	2.284931
H	-6.311163	-4.202405	-1.497820
H	-3.882860	-3.743013	-0.893953
H	-2.417606	-3.075345	0.737946
H	-1.682097	-2.566745	3.004231
H	-3.419160	-2.683502	3.694244
H	-5.993044	0.210152	1.134611
H	-9.458840	-0.202243	-1.254473
H	-5.440024	2.002760	1.971147
H	-7.419958	4.415346	-2.187546
H	-7.172575	5.577545	-0.854129
H	-6.172177	4.044452	-0.992549
H	-11.919702	2.437201	-1.751965
H	-11.337846	0.721729	-1.857496
H	-11.549070	1.412658	-0.264096

Monomer solid 4□7 (BDMB□NVP)

C	-5.311997	-0.022614	-0.127533
C	-5.082972	-1.261383	0.317647
C	-6.109351	-2.049853	0.688843
C	-7.393821	-1.606433	0.619781
C	-7.628057	-0.343820	0.161212
C	-6.572839	0.416544	-0.197249
Br	-3.867880	1.089135	-0.649150
O	-8.378444	-2.490478	1.011268
O	-8.913721	0.139152	0.082144
C	-5.782517	-3.300838	1.133757
O	-6.497409	-4.196528	1.528386
N	-0.692808	1.325242	-0.086731
C	-1.447357	1.460150	-1.099577
C	-0.916037	0.769008	-2.347502
C	-0.002080	-0.287141	-1.729487
C	0.424343	0.401933	-0.425101
C	-0.747589	1.830455	1.079193
C	0.102636	1.659500	2.102553
C	-9.162370	1.461145	-0.335559
C	-9.754624	-2.224934	0.898235
O	-2.482472	2.120440	-1.129077
H	-4.036439	-1.607943	0.369604
H	-6.716275	1.442604	-0.568013
H	-4.687502	-3.525847	1.132361
H	-1.721120	0.331294	-2.978930
H	-0.333588	1.512081	-2.940631
H	0.853468	-0.575549	-2.380546
H	-0.602473	-1.200878	-1.499460
H	0.598859	-0.378607	0.351785
H	1.359675	0.990043	-0.585073
H	-1.607944	2.499900	1.249847
H	-0.076546	2.172017	3.061115
H	1.001967	1.030558	2.054144
H	-10.263144	1.623364	-0.298225
H	-8.686816	2.186522	0.361676
H	-8.833411	1.606373	-1.388654
H	-10.295063	-3.137907	1.236123
H	-10.056425	-1.400938	1.581004

C	5.207503	2.958348	-1.591179	C	9.447876	8.302368	-1.090732
C	5.510937	3.973359	-0.485701	C	8.848234	4.102581	-2.079246
O	3.977786	1.554848	1.448462	C	8.076841	3.028129	-2.340825
C	5.600437	3.728510	1.874311	C	8.474178	1.863080	-1.952166
C	6.399532	4.786720	2.079329	C	9.678180	1.714436	-1.272590
N	5.441186	-1.724290	0.226334	C	10.461362	2.781982	-1.093075
C	4.909210	-2.206699	-0.822065	C	9.974692	4.015992	-1.364380
C	5.504110	-1.662530	-2.113656	Br	8.306922	5.850327	-2.678897
C	6.830897	-1.083727	-1.628075	Br	11.008511	5.546030	-0.984521
C	6.518178	-0.772114	-0.158252	Br	7.388552	0.341428	-2.220691
O	4.000714	-3.034063	-0.857200	Br	10.319354	0.183533	-0.388646
C	5.209521	-1.914249	1.462654	C	6.386252	4.848513	2.672811
C	5.790298	-1.331690	2.522385	C	5.398816	4.584647	1.778770
N	-5.096766	-4.397277	0.295841	C	5.794382	3.900437	0.705445
C	-5.247572	-3.274427	-0.278926	N	6.907721	3.351828	0.476851
C	-6.267008	-2.370043	0.399854	C	7.797975	3.572228	1.351390
C	-7.034480	-3.366194	1.265947	C	7.637006	4.417136	2.392839
C	-5.977857	-4.456169	1.493659	C	1.108494	8.776662	-2.189184
O	-4.653624	-2.911247	-1.291103	C	5.238737	4.951315	4.840185
C	-4.356600	-5.393813	0.018238	C	0.502253	7.374955	-1.978284
C	-4.219725	-6.548040	0.687935	C	-0.297787	6.919051	-3.239373
N	-4.986012	3.169312	-0.586806	C	0.075486	5.557658	-3.774124
C	-5.186133	2.079914	0.035297	C	1.229606	5.233825	-4.347225
C	-6.171498	1.149782	-0.658911	C	1.465852	3.971381	-4.784969
C	-6.876107	2.108012	-1.616435	N	0.590344	3.064345	-4.747467
C	-5.794992	3.175486	-1.835724	C	-0.553780	3.357829	-4.306997
O	-4.660194	1.768611	1.100964	C	-0.837147	4.565705	-3.742931
C	-4.249352	4.170514	-0.316865	C	2.401786	1.495566	-0.798211
C	-4.057728	5.287105	-1.035132	C	2.857502	0.716134	0.156216
H	-0.344906	-2.814625	-1.055286	C	3.069730	-0.582295	-0.056822
H	-0.360375	1.489350	1.249657	C	2.855764	-1.120471	-1.300903
H	4.027829	1.139902	-1.337112	C	2.391846	-0.348426	-2.293494
H	3.087270	2.703750	-1.187277	C	2.095886	0.948866	-1.981293
H	4.957899	3.426435	-2.569777	Br	2.017096	3.324827	-0.465354
H	6.078118	2.272935	-1.733071	Br	1.343696	1.946293	-3.505030
H	6.592230	4.237835	-0.544955	Br	3.709438	-1.496073	1.592649
H	4.889729	4.892127	-0.611812	Br	3.210215	-2.882172	-1.790204
H	5.295888	3.166482	2.773688	C	4.548125	-7.442899	-0.134206
H	6.718492	5.047229	3.101231	C	5.215592	-6.946880	-1.431155
H	6.767448	5.446328	1.282040	C	6.443444	-6.041393	-1.218750
H	5.632759	-2.453629	-2.886046	C	7.277400	-5.839211	-2.465608
H	4.835827	-0.860720	-2.505016	C	8.396458	-4.792029	-2.289795
H	7.169477	-0.194744	-2.206311	C	7.718452	-3.410987	-2.213534
H	7.619021	-1.872869	-1.690591	C	9.296859	-5.016368	-1.139620
H	7.453408	-0.899617	0.434938	C	10.511259	-3.993624	-1.067190
H	6.151549	0.274864	-0.049696	C	11.729977	-4.539467	-0.331939
H	4.417115	-2.651679	1.674363	C	12.557359	-5.562526	-1.192207
H	5.472500	-1.599731	3.542442	C	3.757793	-8.724713	-0.477073
H	6.576965	-0.568485	2.450329	C	3.602542	-6.268368	0.347137
H	-5.728531	-1.623431	1.029114	C	2.460758	-8.776508	-0.966546
H	-6.919151	-1.849362	-0.336576	C	1.846892	-9.954405	-1.122414
H	-7.889097	-3.781407	0.678411	N	2.486894	-11.022321	-0.801974
H	-7.429981	-2.927308	2.209394	C	3.697366	-11.007133	-0.391880
H	-5.376908	-4.234803	2.408010	C	4.362798	-9.888469	-0.131975
H	-6.500422	-5.433048	1.616108	C	7.390593	-2.820544	-1.052130
H	-3.747418	-5.272513	-0.893794	C	6.579099	-1.732192	-1.163365
H	-3.527814	-7.321619	0.318480	N	6.243036	-1.087829	-2.232195
H	-4.755488	-6.787730	1.616296	C	6.547203	-1.746255	-3.310644
H	-5.604002	0.370756	-1.219512	C	7.290549	-2.857696	-3.378406
H	-6.870770	0.669095	0.061208	C	12.960216	-4.987575	-2.586828
H	-7.758142	2.559825	-1.100863	C	13.617175	-3.853030	-2.744772
H	-7.221537	1.626193	-2.558608	C	13.927599	-3.235891	-3.952267
H	-5.144291	2.902710	-2.700822	N	13.575360	-3.865118	-5.030994
H	-6.297402	4.149852	-2.037169	C	13.030620	-4.989753	-4.951326
H	-3.695795	4.089545	0.634288	C	12.652559	-5.533645	-3.783068
H	-3.377654	6.071067	-0.665584	C	2.705445	-6.517503	1.589932
H	-4.535586	5.484276	-2.004192	C	13.682442	-6.104360	-0.321719

Polymer P(5-6) (P(4BB-4VP)) (linker/monomer unit ratio = 1/2)

C	3.499133	9.369302	-1.195222	C	4.707625	-1.947754	3.068427
C	4.155239	9.458831	0.245524	C	3.890906	-2.741507	3.689003
C	5.620391	10.088714	0.329661	C	3.719243	-4.090761	3.610455
C	6.918511	9.297121	-0.087588	C	5.466196	3.421921	5.144068
C	7.880014	8.800526	0.935912	C	6.701350	3.271905	6.120400
C	9.167021	8.344218	0.230030	C	7.170092	1.814826	6.369909
C	7.289290	7.604630	1.709068	C	14.628380	-6.857764	-1.192114
C	6.893505	8.018132	3.138803	C	15.648187	-7.676690	-0.380751
C	5.741152	7.134892	3.724494	C	15.062055	-9.002050	0.293204
C	6.229100	5.677860	3.922626	C	7.806023	1.265304	5.164170
C	4.077465	8.158761	-1.971491	C	14.251597	-8.923784	1.547475
C	1.994114	9.274548	-1.001983	C	9.104814	1.527544	4.947214
C	3.842234	6.841494	-1.588028	C	9.759933	1.083222	3.813971
C	4.364578	5.889710	-2.363723	N	9.160773	0.442137	2.910822
N	5.026575	6.022886	-3.418884	C	7.877194	0.345851	3.027666
C	5.228245	7.179088	-3.807104	C	7.233284	0.546322	4.196666
C	4.740676	8.259300	-3.117852	C	13.058545	-9.546385	1.585216
C	10.171889	8.045183	1.072966	C	12.400553	-9.623632	2.699705
C	11.289128	7.452566	0.598522	N	12.718026	-9.082166	3.798180
N	11.533283	7.326419	-0.657829	C	13.944752	-8.674659	3.871969
C	10.697614	7.899681	-1.434792	C	14.678876	-8.544416	2.782070

C	11.658600	-3.342710	4.044657	H	6.123676	-5.119324	-0.773322
C	11.985368	-4.654417	4.037668	H	6.567756	-5.545667	-3.305882
C	11.145316	-5.688908	3.913896	H	7.741717	-6.828962	-2.810121
C	9.916642	-5.424859	3.466207	H	9.015556	-4.611159	-3.236947
C	9.551554	-4.134582	3.362922	H	8.743418	-4.993771	-0.142554
C	10.347819	-3.081946	3.668376	H	9.703349	-6.058791	-1.105460
Br	12.820581	-1.883076	4.328976	H	10.713157	-3.925359	-2.111288
Br	9.671181	-1.263036	3.362984	H	10.179889	-3.024349	-0.797286
Br	11.822944	-7.496135	3.939710	H	12.417229	-3.696688	-0.056920
Br	8.703656	-6.688888	2.774762	H	11.389249	-4.859941	0.701535
H	3.689581	10.295684	-1.781586	H	11.913339	-6.451777	-1.451985
H	3.529155	10.092241	0.856746	H	4.284147	-5.410111	0.611154
H	4.333612	8.515269	0.734669	H	2.907999	-5.964025	-0.475889
H	5.488960	11.033747	-0.252607	H	1.976515	-7.864170	-1.233566
H	5.824769	10.317942	1.431141	H	0.808960	-10.107509	-1.578545
H	6.570172	8.510459	-0.810752	H	4.187845	-11.960683	-0.239838
H	7.498804	10.076081	-0.697147	H	5.363542	-9.914754	0.185460
H	8.217087	9.555439	1.590699	H	7.575171	-3.095101	0.022861
H	6.464602	7.079980	1.182675	H	6.181369	-1.298836	-0.195363
H	7.918982	6.721607	1.717915	H	5.999969	-1.378781	-4.214652
H	7.772575	8.116640	3.821456	H	7.440079	-3.356308	-4.326263
H	6.380834	8.980211	3.104842	H	13.966293	-3.298934	-1.809414
H	5.423226	7.423017	4.716273	H	14.478451	-2.315819	-4.077081
H	4.794535	7.184702	3.148612	H	12.786367	-5.381367	-5.936767
H	7.181310	5.552125	4.525545	H	12.128887	-6.526178	-3.829699
H	1.694662	10.348654	-0.752668	H	2.211522	-5.540173	1.842323
H	1.604676	8.583197	-0.185546	H	1.902332	-7.324734	1.297408
H	3.357086	6.512578	-0.644863	H	13.243955	-6.544832	0.635636
H	4.204992	4.796198	-2.078265	H	14.189577	-5.207522	0.115803
H	5.985916	7.477534	-4.555257	H	2.883215	-7.236619	3.578931
H	4.998946	9.254525	-3.519558	H	3.817020	-8.105885	2.519911
H	10.081747	8.055993	2.135009	H	5.031417	-6.431925	4.133020
H	12.031118	6.978102	1.263743	H	5.536255	-6.571290	2.370367
H	10.957491	8.103879	-2.546805	H	6.514639	-4.466185	1.816017
H	8.689571	8.666453	-1.900532	H	6.396137	-1.968681	2.162706
H	7.081689	3.100795	-2.817064	H	3.309235	-2.256103	4.492423
H	11.425886	2.666787	-0.533223	H	3.005867	-4.766670	4.197454
H	4.396798	4.995767	1.884641	H	4.550149	2.936809	5.537520
H	5.017621	3.660463	-0.026696	H	5.598574	2.910441	4.150733
H	8.817301	3.054516	1.175797	H	7.473149	3.977079	5.779734
H	8.491997	4.619688	3.065283	H	6.238445	3.756771	7.081025
H	1.593626	8.769071	-3.125718	H	6.211653	1.185315	6.575550
H	0.377998	9.546017	-2.427496	H	7.717585	1.757633	7.426808
H	5.118762	5.350836	5.853867	H	14.049515	-7.559840	-1.774050
H	4.304965	5.162766	4.372664	H	15.173391	-6.165328	-1.862906
H	-0.203255	7.224907	-1.050818	H	16.297578	-8.145814	-1.204803
H	1.342888	6.663623	-1.832754	H	16.303862	-7.162614	0.301466
H	-1.374838	7.074231	-2.901769	H	14.623026	-9.611926	-0.516703
H	-0.003004	7.645865	-4.039876	H	16.049859	-9.484177	0.568922
H	2.019708	5.995231	-4.413694	H	9.676135	2.132911	5.575343
H	2.399438	3.715148	-5.307141	H	10.868146	1.393230	3.647094
H	-1.341124	2.566915	-4.187064	H	7.319725	0.074995	2.090919
H	-1.885508	4.781381	-3.366288	H	6.128400	0.512385	4.277630
H	3.140241	1.326379	1.057791	H	12.626244	-10.154626	0.746758
H	2.266082	-0.544467	-3.355265	H	11.458124	-10.287814	2.671779
H	5.271143	-7.651770	0.646155	H	14.300833	-8.487568	4.859048
H	4.458578	-6.348767	-2.054050	H	15.686387	-8.314086	2.837337
H	5.512229	-7.810842	-2.042125	H	13.019664	-4.867761	4.358449
H	7.011927	-6.495873	-0.360647	H	8.468577	-3.895534	3.121643

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