# **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

Hong Tho Le<sup>1</sup>, Chelsea Violita Stanley<sup>1</sup>, Atsushi Goto<sup>1</sup>

<sup>1</sup> School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, 62 Nanyang Drive, 637459 Singapore (Singapore)

## 1. Materials

trans-4,4'-Dibromostilbene (95%, Sigma-Aldrich, (DBSB) USA), 2,5dibromoterephthalaldehyde (DBTPA) (>97%, Tokyo Chemical Industry (TCI), Japan), trans-4-bromocinnamaldehyde (BCA) (97%, Sigma-Aldrich), 5-bromo-2,3dimethoxybenzaldehyde (BDMB) (97%, Sigma-Aldrich), 1,2,4,5-tetrabromobenzene (4BB) (97%, Sigma-Aldrich), 1,4-diiodotetrafluorobenzene (I-C<sub>6</sub>F<sub>4</sub>-I) (98%, Sigma-Aldrich), 4vinylpyridine (4VP) (95%, Sigma-Aldrich), 1-vinyl-2-pyrrolidone (NVP) (>99%, TCI), 2,2dimethoxy-2-phenylacetophenone (DMPA) (99%, Sigma-Aldrich), ethylene glycol dimethacrylate (EGDMA) (98%, Sigma-Aldrich), dichloromethane (CH<sub>2</sub>Cl<sub>2</sub>) (99.8%, Fisher Scientific, USA), ethanol ( $\geq$ 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)  $\alpha, \alpha, \alpha$ -trifluorotoluene (or trifluoromethylbenzene) (PhCF<sub>3</sub>) ( $\geq$ 99%, Sigma-Aldrich), deuterated chloroform (CDCl<sub>3</sub>) (99.8%D, Cambridge Isotope Laboratories, USA), deuterated dimethyl sulfoxide (DMSO-d<sub>6</sub>) (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  $M_{\rm p} = 46890$ ) (Agilent, US) were used as received.

### 2. Measurement

<sup>1</sup>H NMR spectra were recorded at room temperature on a Bruker (Germany) BBFO400 spectrometer (400 MHz) and AV400 spectrometer (400 MHz). CDCl<sub>3</sub> and DMSO-*d*<sub>6</sub> were used as NMR solvents. The residual non-deuterated solvents were used as the internal standards for <sup>1</sup>H NMR analysis.

The GPC analysis was performed on a Shimadzu (Kyoto, Japan) LC-2030C Plus liquid chromatograph equipped with two Shodex LF-804 columns ( $300 \times 8.0$  mm; bead size = 6  $\mu$ m; pore size = 1500 Å) and one Shodex KD-802 column ( $300 \times 8.0$  mm; bead size = 6  $\mu$ m; 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 ( $\pm$  10) nm wavelength, 900 mW/cm<sup>2</sup>, 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<sup>-1</sup> 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 ( $\lambda_{ex}$ ) = 488 nm and emission wavelength ( $\lambda_{em}$ ) = 493–635 nm)

and a blue laser filter ( $\lambda_{ex} = 405 \text{ nm}$  and  $\lambda_{em} = 410-585 \text{ nm}$ ). The emission intensities were analyzed using Zeiss ZEN blue software at  $\lambda_{em} = 564 \text{ nm}$  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 CuK<sub> $\alpha$ </sub> radiation ( $\lambda$  = 1.541874 Å). The parameters (2theta (2 $\theta$ )) 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 ( $\varepsilon$ ), crystallite size (D), and dislocation density ( $\delta$ ) were calculated from the following formula:

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

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

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

$$\operatorname{Microstrain}\left(\varepsilon\right) = \frac{\operatorname{radians}(\mathrm{FWHM})}{4\tan\theta} \tag{4}$$

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

Where:

## $\beta$ is the radians of FWHM;

 $\theta$  is the incident angle (the angle between the incident ray and the scatter plane) [°];

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

 $\lambda$  is the radiation wavelength ( $\lambda = 0.1541874$  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 Procedures<sup>1</sup>

# 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 mmol), 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 ( $1.7.DMPA \cdot EGDMA$ ) 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).

Entry	Linker·M <sup>a</sup>	[M] <sub>0</sub> /[Linker] <sub>0</sub> /[DMPA] <sub>0</sub> <sup>6</sup>	Monomer conversion (%)	$M_{ m p}{}^c$	<i>M</i> <sub>n</sub> <sup>c</sup>	Ð
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

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

<sup>*a*</sup> Combination of linker and monomer. <sup>*b*</sup> Polymerization in the solid phase under UV irradiation ( $\lambda = 365$  nm) at room temperature for 24 h. <sup>*c*</sup> 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 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 pHstandard 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 CH<sub>2</sub>Cl<sub>2</sub> to remove the residual ions adsorbed on the polymer surfaces, quickly dried with a nitrogen (N<sub>2</sub>) 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-diiodotetrafluorobenzene (I–C<sub>6</sub>F<sub>4</sub>–I, 0.1 M) dissolved in CH<sub>2</sub>Cl<sub>2</sub>, trifluoromethylbenzene (PhCF<sub>3</sub>), and dichloromethane (CH<sub>2</sub>Cl<sub>2</sub>) and sonicated for 30 min. The polymer sheets were then taken out of the solutions, rinsed

with CH<sub>2</sub>Cl<sub>2</sub> to remove the residual linker **5** adsorbed on the polymer surfaces, quickly dried with an N<sub>2</sub> 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 CH<sub>2</sub>Cl<sub>2</sub>) 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 CH<sub>2</sub>Cl<sub>2</sub>) (step 13) and mixture 2 contained all linkers 1–5 (0.05 M in CH<sub>2</sub>Cl<sub>2</sub>) (step 14). The re-embedded polymer sheets were then taken out of the solutions, rinsed with CH<sub>2</sub>Cl<sub>2</sub> to remove the residual linker 5 adsorbed on the polymer surfaces, quickly dried with an N<sub>2</sub> 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  $(3\cdot 6)$  (green), and monomer cocrystal solid  $(3\cdot 7)$  (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.



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 S2Powder X-ray diffraction (PXRD) data of pure linkers (1-5), 4-componentmonomer cocrystals of linkers (1-5) and monomers (6-7), and two presentative obtainedpolymers P(5.6) and P(2.7) (Figs. 2 and S6-S8)

Entry	Compound	2θ (°) <sup>a</sup>	FWHM (°) <sup>a</sup>	d <sub>hkl</sub> spacing (nm) <sup>b</sup>	Microstrain (ɛ) <sup>c</sup>	Crystallite (grain) size (D) (nm) <sup>d</sup>	Dislocation density ( ) (nm <sup>-2</sup> ) <sup>e</sup>	$R_{\rm p}$ (%) <sup>f</sup>	Match ratio (%) <sup>g</sup>
		11.09	0.2891	0.797844	0.01299355				
		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	0.4001	0.010033	0.01390924				
		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	0.4/4023	0.00209124				
		21.34	0.0790	0.400143	0.00202831				
		21.34	0.5245	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				
1	XB linker	28.98	0.0790	0.308115	0.00133383	0.075011	1.040076	7.2	NA
1	1	29.23	0.2765	0.305536	0.00462670	0.975911	1.049970	1.2	INA
		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				
		30.99	0.4364	0.231010	0.00340331				
		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				
		52.55	0.5782	0.174214	0.00333430				
		60.01	0.2442	0.154164	0.00438337				
		60.22	0.5378	0.153677	0.00404646				
		67.20	0.2370	0.139311	0.00155646				
		67.97	0.1975	0.137920	0.00127833				
		10.63	0.1093	0.832264	0.00512635				
		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				
		21.73	0.0007	0.408025	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				
2	XB linker	30.19	0.2169	0.296036	0.00350875	0 978576	1 044265	91	NA
2	2	31.11	0.2346	0.287488	0.00367740	0.976576	1.011200	<i></i>	1411
		31.98	0.1580	0.279863	0.00240583				
		32.72	0.1580	0.2/3/01	0.00234845				
		33.09 30.28	0.2403	0.233/39	0.00339916				
		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	0.1/9239	0.00298557				

		54 21	0.1580	0 169205	0.00134693				
		5(.57	0.1200	0.1(2)(04	0.00102175				
		36.37	0.2370	0.162694	0.001921/5				
		57.52	0.4740	0.160231	0.00376830				
		62.36	0.2370	0.148908	0.00170886				
		66 54	0.1545	0 140522	0.00102744				
		00.54	0.1545	0.140352	0.00102744				
		66.75	0.3222	0.140141	0.00213413				
		77.45	0.3160	0.123235	0.00171950				
		10.94	0.1270	0.016100	0.00624172				
		10.84	0.13/9	0.816188	0.006341/2				
		13.99	0.1691	0.633043	0.00601355				
		16.44	0.1758	0.539213	0.00530998				
		17.96	0 1 2 0 5	0.406640	0.00501221				
		17.80	0.1805	0.490049	0.00301221				
		19.73	0.2228	0.449979	0.00559032				
		22.32	0.0010	0.398315	2.2117E-05				
		22 52	0.2160	0 204822	0.00602543				
		22.52	0.5100	0.374023	0.00072545				
		24.12	0.18/9	0.368983	0.00383/41				
		24.34	0.2427	0.365697	0.00491042				
		24.63	0.1295	0.361457	0.0025883				
		25.67	0.2204	0.347044	0.00441241				
		23.07	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				
		20.50	0.1015	0.202400	0.00407215				
		29.54	0.3003	0.302400	0.00497313				
		30.76	0.2985	0.290679	0.00473498				
		32.58	0.2604	0.274845	0.00388805				
		22.05	0.1516	0.271042	0.00222055				
		22.29	0.1510	0.2/1043	0.00222755				
		33.38	0.3506	0.268438	0.00510226				
		33.90	0.4345	0.264439	0.0062205				
		36.11	0.3806	0.248746	0.00509441				
		27.64	0.0276	0.228070	0.00025225				
	XB linker	57.04	0.0270	0.238979	0.00033333				
3	3	37.85	0.3160	0.237701	0.00402145	0.97667	1.048343	5.7	NA
	5	39.23	0.3160	0.229652	0.00386894				
		39.41	0.3160	0 228644	0.00384981				
		40.22	0.0454	0.220011	0.00054102				
		40.22	0.0434	0.224223	0.00034103				
		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	0.4029	0.214102	0.00455261				
		42.21	0.4028	0.214103	0.00455501				
		42.37	0.3898	0.213331	0.00438839				
		42.54	0.2343	0.212518	0.00262619				
		43.36	0.4098	0.208687	0.00449784				
		13.05	0.3160	0.206022	0.003/1607				
		44.10	0.12(7	0.200022	0.00341077				
		44.10	0.1367	0.205356	0.0014/26				
		44.45	0.3160	0.203820	0.00337446				
		45.61	0.3160	0.198902	0.00327926				
		46.21	0.3160	0 106/158	0.00323170				
		40.21	0.0100	0.105055	0.00323177				
		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				
		50.04	0.4740	0.177001	0.00433173				
		54.//	0.23/0	0.16/60/	0.0019962/				
		55.50	0.1975	0.165574	0.00163793				
		72.28	0.1975	0.130720	0.00118003				
		11 57	0.1440	0 764850	0.00620192				
		11.37	0.1440	0.704030	0.00020183				
		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 487070	0.00441527				
		10.10	0.1017	0.4011(7	0.00441527				
		20.60	0.1452	0.43116/	0.00348623				
		20.90	0.0847	0.425046	0.0020038				
		22.42	0.2370	0.396561	0.00521785				
		22.02	0.1516	0 286250	0.00224827				
		23.02	0.1510	0.380339	0.00324837				
		23.70	0.1/3/	0.3/5425	0.00361216				
		24.29	0.0981	0.366439	0.00198901				
		25.46	0.1622	0.349858	0.00313280				
		25.60	0 1450	0 346778	0.00279189				
	VD 1' 1	20.00	0.1737	0.210720	0.002/0107				
4	AB linker	28.73	0.1564	0.310/39	0.00266462	0.978595	1.044224	10	NA
	4	29.40	0.1418	0.303808	0.00235842				- •• •
		30.85	0.1423	0.289851	0.00225033				
		31.09	0.1474	0.287668	0.00231208				
		24.44	0.0402	0.267000	0.000201200				
		54.44	0.0492	0.200415	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				
		26.00	0.1500	0.242020	0.00200333				
		30.99	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	0.21/602	1 14565 05				
		41./0	0.0010	0.216602	1.1430E-03				
		41.84	0.1922	0.215910	0.00219386				
		44.09	0.1585	0.205400	0.00170787				

		45 42	0.1062	0.100600	0.00204657				
		43.42	0.1903	0.199090	0.00204037				
		46.38	0.1385	0.195778	0.00141066				
		46.79	0.1739	0.194158	0.00175386				
		18 21	0 1782	0 188208	0.00172472				
		40.51	0.1783	0.188398	0.001/34/3				
		50.11	0.1829	0.182045	0.00170715				
		52.31	0.1907	0.174895	0.00169438				
		52.00	0.0884	0 172082	0.00077532				
		52.90	0.0884	0.175082	0.00077332				
		53.05	0.1118	0.172628	0.00097735				
		55 64	0.2125	0 165191	0.00175712				
		55.04	0.2125	0.100101	0.00175712				
		58.37	0.16/1	0.158098	0.00130539				
		58.55	0.1059	0.157655	0.00082425				
		50.24	0.1074	0 155082	0.00082425				
		39.24	0.1074	0.133983	0.00082423				
		59.45	0.2401	0.155482	0.00183484				
		59.77	0.3653	0.154726	0.00277360				
		50.02	0.0660	0 154251	0.00040050				
		59.95	0.0000	0.134331	0.00049950				
		60.72	0.1127	0.152530	0.00083950				
		60.88	0.1393	0.152168	0.00103433				
		65 78	0.1116	0 141070	0.00075200				
		05.78	0.1110	0.141970	0.00073299				
		65.96	0.1131	0.141626	0.00076049				
		66.42	0.1708	0.140757	0.00113844				
		66 50	0 1032	0 1/0/30	0.00128358				
		00.39	0.1932	0.140439	0.00128338				
		68.34	0.3438	0.137263	0.00220983				
		72.58	0.1548	0.130254	0.00091984				
		10.15	0.1407	0.7004((	0.00(00(20				
		12.15	0.148/	0./28466	0.00609639				
		18.53	0.2395	0.478840	0.00640607				
		18.81	0 1811	0 471775	0.00477061				
		10.01	0.1011	0.454001	0.004//001				
		19.55	0.2495	0.454081	0.00631904				
		19.96	0.3774	0.444846	0.00935810				
		22.23	0 2370	0 300007	0.00526360				
		22.23	0.2370	0.377707	0.00520500				
		22.53	0.2370	0.39465	0.00519171				
		24.34	0.1930	0.365697	0.00390486				
		25.62	0 3/32	0 347710	0.00658592				
		25.02	0.3432	0.34//10	0.00038392				
		27.02	0.1275	0.330003	0.00231547				
		27.77	0.3039	0.321259	0.00536420				
		28.15	0 2765	0.317008	0.00481200				
		20.15	0.2705	0.317008	0.00401200				
		30.54	0.2020	0.292/22	0.00322846				
		30.73	0.2379	0.290956	0.00377757				
		31 51	0 3076	0 283020	0.00475734				
		51.51	0.3070	0.203727	0.00+/5/5+				
		32.07	0.5677	0.279098	0.00861866				
		32.28	0.0365	0.277330	0.00055033				
		22.20	0.2050	0.264919	0.00566286				
_	XB linker	33.83	0.3930	0.204616	0.00300380				
5	=	34.78	0.2838	0.257947	0.00395387	0.97545	1.050969	12.9	NA
	5	36.66	0.4422	0.245139	0.00582392				
		27.24	0.2050	0.240920	0.00510060				
		57.54	0.3930	0.240850	0.00310009				
		37.70	0.0098	0.238612	0.00012525				
		37.89	0 3950	0 237460	0.00502110				
		20.51	0 4469	0.220000	0.00542941				
		39.31	0.4408	0.228089	0.00342841				
		41.83	0.1580	0.215959	0.00180396				
		42.46	0.1975	0.212900	0.00221829				
		45.80	0.2270	0.107754	0.00244272				
		45.89	0.2370	0.197734	0.00244272				
		46.11	0.2370	0.196861	0.00242972				
		46.81	0.1580	0.194079	0.00159274				
		40.75	0.2506	0 182277	0.00225822				
		49.75	0.2300	0.165277	0.00255855				
		50.05	0.3399	0.182249	0.00317688				
		52.24	0.3308	0.175112	0.00294372				
		52 42	0 1975	0 174553	0.00175055				
		J. T.	0.1770	5.17 1555	0.001/0000				
		E1 70	A 201A	0 127005	0.00007000				
		54.70	0.2819	0.167805	0.00237803				
		54.70 56.37	0.2819 0.3101	0.167805 0.163223	0.00237803 0.00252505				
		54.70 56.37 63.34	0.2819 0.3101 0.5322	0.167805 0.163223 0.146838	0.00237803 0.00252505 0.00376431				
		54.70 56.37 63.34 79.02	0.2819 0.3101 0.5322 0.1975	0.167805 0.163223 0.146838 0.121162	0.00237803 0.00252505 0.00376431				
		54.70 56.37 63.34 79.03	0.2819 0.3101 0.5322 0.1975	0.167805 0.163223 0.146838 0.121163	0.00237803 0.00252505 0.00376431 0.00104484				
		54.70 56.37 63.34 79.03 12.94	0.2819 0.3101 0.5322 0.1975 0.1533	0.167805 0.163223 0.146838 0.121163 0.684165	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829				
		54.70 56.37 63.34 79.03 12.94 19.37	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503				
		54.70 56.37 63.34 79.03 12.94 19.37	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412552	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.383402	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.369284	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00280460				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00308469				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00308469 0.00318658				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038658 0.00318658 0.00335146				
		54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 28.84	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309572	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.00335146 0.00335146				
	Monomer	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975	0.167805 0.163223 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.369284 0.354100 0.344275 0.309578 0.299722	$\begin{array}{c} 0.00237803\\ 0.00252505\\ 0.00376431\\ 0.00104484\\ 0.00589829\\ 0.00462503\\ 0.00390185\\ 0.00576900\\ 0.00380799\\ 0.00308469\\ 0.00318658\\ 0.00335146\\ 0.00323758\\ \end{array}$				
	Monomer	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1975	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.309578 0.299722 0.283054	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038069 0.00318658 0.00323758 0.002250486	0.075/77	1.050494		
6	Monomer cocrystal	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1975 0.1625 0.1692	0.167805 0.163223 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.75751	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.00335146 0.00323758 0.00250486 0.00253337	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1-6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1625 0.1692	0.167805 0.163223 0.163223 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00380799 0.00318658 0.00335146 0.00323758 0.00250486 0.00253337	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1625 0.1692 0.1898	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.00335146 0.00323758 0.00220486 0.00253537 0.00261623	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1.6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.59	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1975 0.1625 0.1692 0.1898 0.2752	0.167805 0.163223 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.252260	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.00335146 0.0023758 0.00250486 0.00250486 0.00253537 0.00261623 0.00374113	0.975675	1.050484	9.4	NA
6	Monomer cocrystal ( <b>1</b> ·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.59 37.83	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1625 0.1692 0.1898 0.2752 0.2316	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.252260 0.37822	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00318658 0.00335146 0.00323758 0.00250486 0.00253337 0.00250486 0.00253337 0.00261623 0.00374113 0.00294004	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13 35.59 37.83 20.17	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1625 0.1692 0.1898 0.2752 0.2316	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.252260 0.237822 0.230929	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.00325146 0.00323758 0.00250486 0.00253537 0.00261623 0.00374113 0.00294904 0.00243065	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1.6)	$\begin{array}{r} 54.70\\ 56.37\\ 79.03\\ 12.94\\ 19.37\\ 21.54\\ 23.20\\ 24.10\\ 25.15\\ 25.88\\ 28.84\\ 29.81\\ 31.61\\ 32.47\\ 35.13\\ 35.59\\ 37.83\\ 39.17\\ \end{array}$	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1692 0.1898 0.2752 0.2316 0.1982	0.167805 0.163223 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.255260 0.237822 0.229990	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00308469 0.00318658 0.00335146 0.00323758 0.00250486 0.00250486 0.00253537 0.00261623 0.00374113 0.00294904 0.00243068	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1.6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13 35.59 37.83 39.17 40.78	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1675 0.1975 0.1625 0.1692 0.1898 0.2752 0.2316 0.1982 0.1691	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.255457 0.252260 0.237822 0.229990 0.221274	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00318658 0.00335146 0.00323758 0.00250486 0.00253537 0.00261623 0.00243068 0.00243068 0.00198505	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13 35.59 37.83 39.17 40.78 43.93	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1675 0.1692 0.1898 0.2752 0.2316 0.1982 0.2316	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.252457 0.252260 0.237822 0.229990 0.221274 0.206111	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00318658 0.0035146 0.00323758 0.00250486 0.00253537 0.00261623 0.00374113 0.00294904 0.00243068 0.00198505 0.00227732	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13 35.59 37.83 39.17 40.78 43.93	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1678 0.1975 0.1678 0.1975 0.1675 0.1675 0.1692 0.1898 0.2752 0.2316 0.1982 0.1691 0.2105	0.167805 0.163223 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.255457 0.255260 0.237822 0.229990 0.221274 0.206111 0.202492	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.0038469 0.00335146 0.00323758 0.00250486 0.00253537 0.00261623 0.00374113 0.00294904 0.00243068 0.00198505 0.00227732 0.00227732	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1·6)	54.70 56.37 63.34 79.03 12.94 19.37 21.54 23.20 24.10 25.15 25.88 28.84 29.81 31.61 32.47 35.13 35.59 37.83 39.17 40.78 43.93 44.76	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1771 0.1678 0.1975 0.1678 0.1975 0.1625 0.1692 0.1898 0.2752 0.2316 0.1982 0.1691 0.2105 0.1794	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.369284 0.354100 0.344275 0.309578 0.299722 0.283054 0.275751 0.255457 0.252260 0.237822 0.229990 0.221274 0.206111 0.202480	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00380799 0.0038469 0.00323758 0.00250486 0.00253537 0.00261623 0.0025486 0.00253537 0.00261623 0.0024904 0.00243068 0.00198505 0.00227732 0.00190105	0.975675	1.050484	9.4	NA
6	Monomer cocrystal (1-6)	$\begin{array}{c} 54.70\\ 56.37\\ 63.34\\ 79.03\\ 12.94\\ 19.37\\ 21.54\\ 23.20\\ 24.10\\ 25.15\\ 25.88\\ 28.84\\ 29.81\\ 31.61\\ 32.47\\ 35.13\\ 35.59\\ 37.83\\ 39.17\\ 40.78\\ 43.93\\ 44.76\\ 45.98\\ \end{array}$	0.2819 0.3101 0.5322 0.1975 0.1533 0.1809 0.1701 0.2714 0.1863 0.1577 0.1678 0.1975 0.1975 0.1975 0.1692 0.1898 0.2752 0.2316 0.1982 0.1691 0.2105 0.1794	0.167805 0.163223 0.146838 0.121163 0.684165 0.458260 0.412559 0.383402 0.369284 0.369284 0.34275 0.309578 0.299722 0.283054 0.245751 0.255457 0.252260 0.237822 0.229990 0.221274 0.26111 0.202480 0.197387	0.00237803 0.00252505 0.00376431 0.00104484 0.00589829 0.00462503 0.00390185 0.00576900 0.00380799 0.00380799 0.0038469 0.00318658 0.00325146 0.00323758 0.00250486 0.00250486 0.00250486 0.00250486 0.00250486 0.00250486 0.00250486 0.00250486 0.002540468 0.00198505 0.00227732 0.00190105 0.00204453	0.975675	1.050484	9.4	NA

		47.02	0.2642	0 102222	0.00265212				
		47.03 52.49	0.3043	0.193223	0.00303312				
		52.48	0.2391	0.172940	0.00229331				
		52.98	0.1324	0.172840	0.00115920				
		53.15	0.1899	0.1/232/	0.0016564/				
		53.49	0.2241	0.1/1312	0.00194038				
		58.75	0.3555	0.157166	0.00275568				
		60.27	0.1/19	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				
		21.25	0.0010	0.407882	2 2669E-05				
		21.79	0.0010	0.207426	0.00201460				
		22.57	0.0715	0.308115	0.00201402				
		20.90	0.4175	0.306113	0.00704902				
	Monomer	30.10	0.16//	0.290900	0.00304390				
7	cocrystal	31.97	0.1433	0.279948	0.00218271	0.980435	1.040309	10.6	NA
	(2.6)	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				
		11.50	0.1096	0.749993	0.00270094				
		12.08	0.1027	0.732671	0.004027631				
		12.00	0.1037	0.752071	0.00427031				
		12.31	0.1304	0.707383	0.00319111				
		14.74	0.1111	0.600997	0.003/4/85				
		15.02	0.0790	0.589856	0.00261475				
		15.43	0.0790	0.5/42/3	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				
	м	18.82	0.1185	0.471526	0.00311989				
0	Monomer	19.04	0.0395	0.466127	0.00102773	0.050(1.4	1.044105		
8	cocrystal	19.76	0.1975	0.449303	0.00494784	0.9/8614	1.044185	6.5	NA
	(3.6)	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				
		21.50	0.1770	0.305516	0.01040711				
		22.40	0.1185	0.378734	0.00248602				
		23.49	0.1185	0.376734	0.00248092				
		25.05	0.0393	0.370200	0.00002320				
		25.15	0.0790	0.243984	0.00130807				
		20.91	0.0393	0.331327	0.000/2039				
		28.12	0.2765	0.31/339	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				

		34.95	0.0395	0 256731	0.00054746				
		34.75	0.0375	0.250751	0.000004740				
		35.10	0.0790	0.255668	0.00108994				
		36.25	0.1975	0.247817	0.00263266				
		36.94	0.0790	0 243345	0.00103200				
		20.05	0.0790	0.245545	0.00105200				
		39.05	0.0790	0.230669	0.0009/206				
		39.75	0.1821	0.226767	0.00219795				
		40.35	0.1502	0 223532	0.00178365				
		41.90	0.1252	0.215((4	0.00154570				
		41.89	0.1356	0.215664	0.001545/8				
		42.24	0.0637	0.213958	0.00071956				
		12 13	0.2148	0 213043	0.00241448				
		42.43	0.2146	0.213043	0.00241446				
		42.93	0.0883	0.210677	0.00097985				
		43.32	0.1580	0.208871	0.00173593				
		12.61	0.0205	0.207540	0.00042080				
		45.01	0.0393	0.207349	0.00043080				
		44.08	0.0790	0.205444	0.00085146				
		44.40	0.0790	0.204038	0.00084467				
		11 58	0.0305	0.203255	0.00042044				
		44.50	0.0575	0.205255	0.00042044				
		44./4	0.0790	0.202566	0.00083/56				
		45.80	0.1185	0.198121	0.00122404				
		45.91	0.1185	0.197672	0.00122077				
		16.88	0.0205	0 103806	0.00020752				
		40.88	0.0395	0.193800	0.00039752				
		47.98	0.0395	0.189616	0.00038729				
		48.57	0.0395	0.187450	0.00038198				
		50.36	0.0305	0 181100	0.00036660				
		50.50	0.0373	0.101177	0.00050000				
		50.76	0.0790	0.1/9865	0.000/2660				
		52.89	0.0395	0.173113	0.00034652				
		54.06	0.0395	0.169639	0.00033782				
		54.01	0.0395	0.167010	0.00033173				
		54.91	0.0395	0.16/213	0.000331/2				
		56.44	0.0790	0.163038	0.00064233				
		56.60	0.0395	0.162615	0.00032009				
		56.00	0.0395	0.161054	0.00032007				
		30.89	0.0395	0.101854	0.00031816				
		57.43	0.0790	0.160460	0.00062922				
		57.71	0.1185	0.159748	0.00093838				
		60.42	0.1492	0.152102	0.00111112				
		60.43	0.1485	0.155195	0.00111115				
		60.61	0.1771	0.152781	0.00132213				
		60.93	0.0194	0.152055	0.00014391				
		61.12	0.1176	0.151605	0 00006006				
		01.15	0.11/0	0.131003	0.00080880				
		62.41	0.0395	0.148800	0.00028453				
		66.55	0.0790	0.140513	0.00052526				
		66.88	0.0700	0.120000	0.00052108				
		00.88	0.0790	0.139900	0.00032198				
		68.31	0.0794	0.137316	0.00051064				
		73.52	0.0790	0.128819	0.00046144				
		75 42	0.1280	0.126025	0.00072721				
		/3.43	0.1289	0.126025	0.00072731				
		75.65	0.1634	0.125713	0.00091832				
		76.78	0.1484	0.124142	0.00081726				
		77.04	0.2108	0 1227299	0.00120484				
		//.04	0.2198	0.125/88	0.00120484				
		77.54	0.1619	0.123114	0.00087955				
		78.08	0.0790	0.122398	0.00042507				
		70.14	0.0205	0.121022	0.00020856				
		/9.14	0.0393	0.121022	0.00020836				
		11.64	0.1194	0.760266	0.00511121				
		11.84	0.0010	0.747468	4.2079E-05				
		12.12	0.1590	0.720662	0.00649942				
		12.15	0.1580	0.729005	0.00048845				
		12.89	0.0790	0.686807	0.00305146				
		16.31	0.1975	0.543482	0.00601363				
		18.26	0 1307	0.485850	0.00354852				
		10.20	0.1307	0.400000	0.00334032				
		20.71	0.1/54	0.428902	0.00418846				
		22.39	0.1406	0.397086	0.00309974				
		22.92	0.0864	0.388022	0.00185961				
		23 11	0 1206	0 384875	0.00276586				
		23.11	0.1270	0.222216	0.002/0500				
		23.81	0.14/4	0.3/3/16	0.00305066				
		24.42	0.1255	0.364517	0.00253060				
		25.70	0.2720	0.346645	0.00520280				
		20.70	0 1227	0.200054	0.00220200				
		20.09	0.1327	0.309034	0.00224//8				
	Monomer	29.50	0.1334	0.302801	0.00221085				
0		30.92	0.1496	0.289211	0.00236015	0.07777	1.046405	0.7	
9	cocrystal	31.15	0 1402	0 287128	0.00233558	0.977574	1.046407	8.6	NA
	(4.6)	24.54	0.1772	0.20/120	0.002333330				
	< - /	34.54	0.1269	0.259684	0.00178103				
		34.82	0.1602	0.257660	0.00222916				
		35.30	0.1459	0.254265	0.00200079				
		26 71	0 1557	0.227203	0.00200077				
		30./1	0.155/	0.24481/	0.00204/63				
		37.14	0.1400	0.242081	0.00181830				
		38.94	0.2998	0.231295	0.00370019				
		11 22	0 1029	0.210012	0.00222402				
		+1.22	0.1928	0.219013	0.00223092				
		41.83	0.1998	0.215959	0.00228121				
		42.13	0.3110	0.214491	0.00352314				
		42 50	0.2765	0.212709	0.00310240				
		45.50	0.1240	0.212/07	0.00120740				
		45.59	0.1346	0.198985	0.00139/48				
		46.44	0.2345	0.195539	0.00238500				
		46.89	0.4121	0.193767	0.00414629				
		10.05	0 2012	0 100060	0.00105242				
		48.40	0.2012	0.188069	0.00195342				
		49.71	0.1545	0.183415	0.00145529				

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		50.23	0 2333	0 181638	0.00217164				
		50.25	0.2555	0.174522	0.00217104				
		52.45	0.1580	0.174323	0.00140015				
		53.00	0.0790	0.172779	0.00069137				
		55.77	0.1462	0.164836	0.00120558				
		59.04	0 1277	0 156463	0.00098404				
		50.20	0.0294	0.156079	0.00057800				
		59.20	0.0884	0.150078	0.00007899				
		59.56	0.1486	0.155221	0.00113307				
		59.75	0.1360	0.154773	0.00103302				
		60.84	0 1147	0 152258	0.00085235				
		60.07	0.1072	0.151065	0.00146227				
		60.97	0.19/3	0.131963	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				
		00.40	0.1075	0.140044	0.00103172				
		00.00	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 1222	0 721465	0.00548778				
		12.10	0.1333	0.731403	0.00348778				
		17.60	0.3235	0.503927	0.00911/96				
		18.51	0.2575	0.479353	0.00689510				
		18.79	0.182	0.472272	0.00479952				
		10.48	0.2480	0.455607	0.00632604				
		10.00	0.2469	0.445720	0.00032074				
		19.92	0.3552	0.445/30	0.00882568				
		22.05	0.5802	0.403131	0.01299368				
		22.40	0.4581	0.396911	0.01009487				
		22.06	0 2265	0 287255	0.00508116				
		22.90	0.2303	0.367333	0.00308110				
		24.30	0.1814	0.366290	0.0036/639				
		25.68	0.1239	0.346911	0.00237186				
		26.49	0.3000	0.336484	0.00556129				
		27.03	0.1161	0 320883	0.00210763				
		27.05	0.1101	0.327003	0.00210703				
		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				
		20.74	0.1950	0.202007	0.007/79091				
		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				
		22.95	0.4710	0.264010	0.00675262				
		33.83	0.4/10	0.204818	0.000/3362				
	Monomer	34.31	0.0870	0.261372	0.00122974				
10	cocrystal	34.67	0.4375	0.258740	0.00611578	0.974161	1.05375	9.0	NA
	(5.6)	36.52	0 2370	0 246047	0.00313419				
	( <b>30</b> )	27.25	0.2270	0.241201	0.00206926				
		37.23	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				
		20.42	0.2270	0.2200077	0.00299577				
		39.43	0.2370	0.228333	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				
		12 25	0.4384	0.200102	0.00482523				
		45.50	0.2270	0.207172	0.00402525				
		45.59	0.23/0	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 10/511	0.00230541				
		40.70	0.1907	0.102212	0.00237341				
		49./4	0.180/	0.103312	0.001/0091				
		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				
		62.74	0.0047	0.145072	0.00230302				
		03./0	0.064/	0.1459/2	0.00045390				
		63.89	0.3923	0.145706	0.00274520				
		74.18	0.1185	0.127836	0.00068392				
		78 16	0 1975	0 122202	0.00106115				
		/0.10	0.17/3	0.122292	0.00100113				
		12.09	0.1588	0.732068	0.00654302				
		17.63	0.1805	0.503076	0.00507866				
		17.82	0.0763	0 497755	0.00212357				
		10.42	0.0705	0.401.414	0.00212557				
		18.43	0.3036	0.481416	0.00816543				
		18.75	0.2268	0.473271	0.00599393				
		19.49	0.2730	0.455466	0.00693593				
		10.99	0 3029	0 116618	0.00080486				
		19.00	0.3938	0.440018	0.00900480				
	Polymer	21.79	0.4740	0.407882	0.01074514				55%
11	B/F C	21.99	0.0719	0.404217	0.00161472	0.976107	1.049554	10.1	(21/50)
	P(5·6)	22.25	0.5394	0.399552	0.01196863				(31/36)
		22 75	0 2302	0 300893	0.00/00260				
		22.13	0.2502	0.370003	0.00477207				
		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				
		20.21	0.2034	0.010047	0.0073/300				
		30.48	0.2159	0.293285	0.00345775				
		30.66	0.2240	0 291604	0.00356538				

		21.42	0.2214	0.284624	0.00408400				
		31.43	0.3214	0.204034	0.00498409				
		31.94	0.4/56	0.280204	0.00/25140				
		33.55	0.2237	0.267117	0.00323802				
		33.91	0.2498	0.264363	0.00357513				
		24.22	0.2242	0.262030	0.00450676				
		34.22	0.3243	0.202039	0.00439070				
		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				
		27.20	0.3923	0.240307	0.007094062				
		37.20	0.2993	0.241/04	0.00388033				
		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	0.1195	0.2220120	0.00120779				
		40.00	0.1185	0.222215	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				
		49.07	0.2370	0.103337	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				
		03.23	0.5100	0.14/023	0.00223903				
		09.01	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 1974	0.440261	0.00460224				
		20.17	0.18/0	0.440201	0.00400234				
		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	0.2001	0.354100	0.00400000				
		25.15	0.2091	0.334100	0.00409009				
		25.96	0.1438	0.343232	0.002/2210				
		26.41	0.0012	0.337485	2.2315E-05				
		28.92	0.3042	0.308740	0.00514720				
		20.86	0.1766	0 200232	0.00288000				
		29.80	0.1700	0.299232	0.00288990				
		31.70	0.1919	0.2822/1	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				
		27.95	0.2555	0.227701	0.00250550				
		57.85	0.3333	0.237701	0.00432413				
	Monomer	38.52	0.2765	0.233720	0.00345283				
10	accomutatel colid	39.24	0.1975	0.229596	0.00241742	0.07707(	1.04576	0.4	NT A
12	cocrystal solid	40.31	0.2370	0.223745	0.00281745	0.9//8/6	1.04576	9.4	NA
	1.7	40.84	0.1185	0.220063	0.00128882				
		40.84	0.1105	0.220903	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				
		47.00	0.1415	0.102000	0.00300077				
		47.09	0.1415	0.192990	0.00141090				
		50.31	0.3090	0.181368	0.00287106				
		52.57	0.1648	0.174091	0.00145590				
		53.08	0.1842	0.172538	0.00160921				
		52 56	0 2211	0.171104	0.00101150				
		60.25	0.2211	0.1/1104	0.00110571				
		00.35	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				
		67.00	0.1402	0 127004	0.00111412				
		67.99	0.1692	0.13/884	0.001094/4				
		75.63	0.1493	0.125741	0.00083938				
		75.84	0.1663	0.125445	0.00093143				
		10.91	0 1245	0.818446	0.00620262				
		10.01	0.1343	0.018440	0.00020203				
		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 50	0.1044	0 /1100/	0.00220024				
		21.30	0.1044	0.411004	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 323880	0.00323686				
	Ma	21.34	0.1010	0.323009	0.00323080				
	Monomer	28.82	0.1770	0.309789	0.00300576				
13	cocrystal	29.65	0.0894	0.301303	0.00147379	0.977219	1.047167	6.9	NA
	cocrystal (2·7)	30.06	0.1929	0.297286	0.00313465				
		20.00	0.1/2/	0 282401	0.00255281				
		31 56	0.1654	0.203471	0.00233361				
	(2.7)	31.56	0.1654	0.075000	0.00170400	31 99 48			
	(2.7)	31.56 32.52	0.1654 0.1006	0.275338	0.00150499				
	(2.7)	31.56 32.52 34.87	0.1654 0.1006 0.1722	0.275338 0.257302	0.00150499 0.00239248				
	(2.7)	31.56 32.52 34.87 35.27	0.1654 0.1006 0.1722 0.1620	0.275338 0.257302 0.254475	0.00150499 0.00239248 0.00222359				
	(2.7)	31.56 32.52 34.87 35.27 36.26	0.1654 0.1006 0.1722 0.1620 0.1145	0.275338 0.257302 0.254475 0.247751	0.00150499 0.00239248 0.00222359 0.00152582				
	(2.7)	31.56 32.52 34.87 35.27 36.26	0.1654 0.1006 0.1722 0.1620 0.1145	0.275338 0.257302 0.254475 0.247751	0.00150499 0.00239248 0.00222359 0.00152582				
	(2.7)	31.56 32.52 34.87 35.27 36.26 37.48	0.1654 0.1006 0.1722 0.1620 0.1145 0.2040	0.275338 0.257302 0.254475 0.247751 0.239962	0.00150499 0.00239248 0.00222359 0.00152582 0.00262371				
	(2.7)	31.56 32.52 34.87 35.27 36.26 37.48 39.8	0.1654 0.1006 0.1722 0.1620 0.1145 0.2040 0.1832	0.275338 0.257302 0.254475 0.247751 0.239962 0.226493	0.00150499 0.00239248 0.00222359 0.00152582 0.00262371 0.00220821				
	(2.7)	31.56 32.52 34.87 35.27 36.26 37.48 39.8 41.22	0.1654 0.1006 0.1722 0.1620 0.1145 0.2040 0.1832 0.2568	0.275338 0.257302 0.254475 0.247751 0.239962 0.226493 0.219013	0.00150499 0.00239248 0.00222359 0.00152582 0.00262371 0.00220821 0.00297947				

		44 51	0.2501	0 203559	0.00266675				
		45.57	0.2301	0.205555	0.00200075				
		43.37	0.2736	0.19906/	0.00284205				
		46.82	0.2584	0.194040	0.00260421				
		48.06	0.2782	0.189319	0.00272257				
		50.20	0.4278	0 181739	0.00398483				
		50.26	0.2092	0.170525	0.00101151				
		50.80	0.2085	0.179353	0.00191131				
		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				
		55.05	0.1020	0.105105	0.00004020				
		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	0.148051	0.002/11185				
		02.34	0.4730	0.140951	0.00341185				
		65.74	0.3927	0.14204/	0.00265168				
		65.96	0.1064	0.141626	0.00071544				
		10.71	0.2780	0.826066	0.01294071				
		1/ 03	0 1/05	0 503301	0.00/0783/				
		15.00	0.1510	0.575571	0.00497034				
		15.66	0.1519	0.565890	0.004819/1				
		20.79	0.1049	0.427270	0.00249511				
		22.38	0.1899	0.397261	0.00418855				
		23.76	0.2418	0.374491	0.00501525				
		24.40	0.0000	0 262/01	0.00180042				
		24.49	0.0900	0.303491	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				
		29.80	0.2150	0.300000	0.00365371				
		28.80	0.2130	0.309999	0.00303371				
		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				
		22.22	0.1942	0.26920	0.003/7070				
		33.33	0.1845	0.208830	0.00208037				
		35.33	0.1466	0.254056	0.00200856				
		36.21	0.2312	0.248082	0.00308552				
		36.75	0.2069	0.244559	0.00271779				
		37 /3	0.3035	0.240271	0.00300001				
14	Polymer	20.82	0.3033	0.2402/1	0.00320201	0.076925	1.049012	05	58 %
14	$P(2\cdot7)$	39.82	0.1920	0.226384	0.00231302	0.976825	1.048013	8.5	(28/48)
	- (- /)	41.34	0.1881	0.218405	0.00217547				(20, 10)
		42.23	0.3570	0.214006	0.00403375				
		43 70	0 2415	0 207142	0.00262789				
		14 54	0.2848	0.202420	0.00202/09				
		44.34	0.2040	0.203429	0.00303448				
		45./4	0.3080	0.19836/	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				
		47.06	0.4175	0.190601	0.001000001				
		47.90	0.4173	0.169091	0.00409342				
		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				
		56.80	0.1195	0.161954	0.00105379				
		50.89	0.1165	0.101654	0.00093448				
		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				
		71.99	0.1590	0 131340	0.00005008				
		71.00	0.1500	0.131347	0.00075078				
		/3.10	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				
		12.00	0.1050	0 (27570	0.007012002				
		13.89	0.1958	0.03/5/8	0.00/01368				
		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				
		17.05	0.2590	0 40/170	0.00715538				
		10.00	0.2390	0.4241/9	0.00/13330				
	Monomer	19.80	0.2849	0.448404	0.00/122/0				
15	coervetal	20.27	0.5999	0.438112	0.01464307	0 978081	1 045323	73	NA
15	cocrystar	22.63	0.2671	0.392929	0.00582454	0.7/0001	1.043323	1.5	INA
	(3.7)	23.05	0.2523	0.385863	0.00539887				
		20.00	0 2275	0.260000	0.00337007				
		24.0/	0.23/3	0.300880	0.004/3894				
		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 317803	0 00435674				
		20.07	0.2770	0.212400	0.00446164				
		28.48	0.2595	0.313409	0.00446164				
		-							

10         0.2014         0.2019         0.0033099           10.33         0.2017         0.0073473         0.0073473           13.34         0.2017         0.0073473         0.0073473           13.34         0.2170         0.006399         1           13.34         0.1757         0.207401         0.0022319           13.34         0.1767         0.27640         0.004609           13.34         0.2764         0.0054007           13.34         0.2764         0.0054007           13.34         0.2764         0.0054071           13.34         0.2764         0.0054071           14.34         0.2764         0.0034027           14.35         0.2765         0.0034027           14.34         0.167         0.0034027           14.34         0.167         0.003477           14.34         0.167         0.003477           14.34         0.167         0.003477           14.34         0.167         0.004577           14.34         0.167         0.004577           14.34         0.167         0.005746           14.34         0.167         0.005746           14.34         0.1185										
16         Memory         0.23210         0.02780/62           16         0.2531         0.25471         0.027471         0.00739/73           17         0.027471         0.00739/73         0.00739/73           18         0.0714         0.024590         0.0025379           18.15         0.0214590         0.0025379           18.15         0.0214590         0.0025379           18.15         0.0214590         0.0021494           18.16         0.12155         0.0021494           18.16         0.12154         0.0023607           18.16         0.12155         0.0023607           18.16         0.12154         0.0023607           18.18         0.1161         0.222341         0.0023607           18.18         0.1161         0.022341         0.0023607           18.18         0.1161         0.0021507         1.116           18.18         0.1161         0.0021503         0.002364           18.18         0.1161         0.0071941         1.116           18.19         0.27581         0.002544         1.116           18.19         0.27681         0.0071941         1.116           18.19         0.2764			29.71	0.2024	0.300708	0.00332959				
14         32,235         0.0020         0.278.909         2.0046-05           32,245         0.2507         0.272.17         0.0063399           33,34         0.160         0.270531         0.0023399           33,24         0.310         0.270531         0.0023399           33,24         0.310         0.247053         0.0023704           33,34         0.3160         0.230216         0.0037061           33,34         0.3160         0.230214         0.0013163           34,34         0.3160         0.230214         0.0013163           42,25         0.1169         0.0012159         0.0022566           42,35         0.24169         0.0002256         0.23163           42,38         0.4749         0.230523         0.0022566           44,38         0.4749         0.230523         0.0022566           44,38         0.4749         0.0022566         0.0022566           44,38         0.3766         0.002138         0.0022566           45,38         0.3766         0.002138         0.002138           45,38         0.3766         0.002138         0.001136           45,48         0.3566         0.002136         0.00166			30.52	0 4883	0 292910	0.00780962				
14         9.253         0.2572         0.0073443           33.14         0.1575         0.257344         0.00228.39           3.264         0.3160         0.27383         0.00421.49           3.264         0.3160         0.27383         0.00421.49           3.264         0.3160         0.23783         0.0032057           3.264         0.3160         0.23784         0.0033027           3.264         0.2375         0.22324         0.0033027           4.035         0.3160         0.23784         0.0033027           4.035         0.3160         0.23784         0.0039784           4.437         0.358         0.014971         0.0035784           4.438         0.3160         0.23784         0.003784           4.458         0.3160         0.2754         0.0035786           4.459         0.3506         0.003784         0.003784           4.459         0.3506         0.003784         0.003784           4.459         0.3506         0.003784         0.003784           4.459         0.3506         0.003784         0.003784           4.590         0.2756         0.1758         0.003784           4.590 <td< td=""><td></td><td></td><td>22.12</td><td>0.4005</td><td>0.272500</td><td>2.0204E.05</td><td></td><td></td><td></td><td></td></td<>			22.12	0.4005	0.272500	2.0204E.05				
16         12,153         0.2000         0.219471         0.0021349           13,55         0.0575         0.020539         0.022339           13,58         0.674         0.23590         0.0025079           13,73         0.4740         0.23593         0.0021149           13,73         0.4740         0.23543         0.0021507           14,013         0.1975         0.22544         0.0023675           14,013         0.1975         0.22543         0.0023675           14,215         0.3558         0.21494         0.0023675           14,215         0.3555         0.215149         0.0023675           14,328         0.4749         0.0023566         1.111           14,328         0.4749         0.0023566         1.111           14,328         0.4749         0.0023566         1.111           14,328         0.3160         0.11714         0.002254           14,328         0.2765         0.11748         0.002264           14,328         0.2766         0.11748         0.0026173           14,329         0.2766         0.11748         0.0026424           14,429         0.1169         0.152540         0.0021134			32.13	0.0020	0.278390	5.0304E-05				
14         0.3160         0.270127         0.0026339           33.30         0.571         0.27933         0.0092134           33.31         0.160         0.27933         0.0092134           37.63         0.160         0.27034         0.0083706           39.50         0.2705         0.221344         0.0033007           40.03         0.1075         0.223344         0.0033007           40.33         0.1075         0.223444         0.003507           42.21         0.1185         0.210494         0.0002516           42.27         0.1185         0.210499         0.0013163           43.84         0.4760         0.203579         0.0032509           44.38         0.4760         0.0025245         0.0032509           46.35         0.3593         0.191231         0.0032509           47.66         0.4545         0.189630         0.0012218           47.66         0.4545         0.189761         0.002134           47.66         0.4545         0.189761         0.0021131           47.66         0.4576         0.0021131         0.0034431           47.66         0.4576         0.0021473         0.0024441           51.61 <td></td> <td></td> <td>32.65</td> <td>0.2507</td> <td>0.274271</td> <td>0.00373475</td> <td></td> <td></td> <td></td> <td></td>			32.65	0.2507	0.274271	0.00373475				
14         8.3.00         0.1575         0.267340         0.00228339           31.8.8         0.3164         0.3160         0.247833         0.0031037           31.3.1         0.1575         0.228140         0.0031027         0.0031047           31.3.1         0.1755         0.228140         0.0031027         0.218140         0.0031017           40.05         0.3160         0.228243         0.0037141         0.0031017         1.0017141           41.3.8         0.3160         0.228243         0.0037141         0.003111         1.0017141           41.3.8         0.1160         0.238140         0.0011317         1.0017147         1.0027866           41.4.8         0.1160         0.238150         0.0014777         1.0027866         1.001147           41.4.8         0.1560         0.002234         1.0017866         1.0027866         1.001786           41.4.8         0.1560         0.002244         1.0017866         0.002124         1.001786         1.001786           41.4.8         0.1560         0.002124         1.001786         0.001713         1.001786           51.4.9         0.1576         0.15786         0.0011141         1.001786         1.001787           51.4.9			33.14	0.3160	0.270327	0.00463399				
14         3388         0.0674         0.024590         0.0095079           36.24         0.1606         0.239940         0.0007013         0.0035027           39.33         0.1616         0.23144         0.0035027         0.0035027           40         0.160         0.23144         0.0035027         0.0035027           40         0.160         0.23144         0.003502         0.003502           41.45         0.155         0.214940         0.0002516         0.0013502           42.97         0.155         0.214940         0.0002516         0.0014977           43.88         0.166         0.23150         0.002506         0.0014977           43.89         0.167         0.18502         0.002506         0.0014977           44.58         0.1676         0.18630         0.002202         0.002506           51.91         0.16716         0.002505         0.001134         0.0014911           45.83         0.1670         0.002505         0.0021302         0.002506           51.91         0.168716         0.0021302         0.168716         0.0021302         0.168716           52.91         0.15716         0.15716         0.0025013         0.168716         0.00			33 50	0 1575	0 267504	0.00228339				
13.8.3         0.0749         0.24793         0.0002103           37.6.3         0.4749         0.230014         0.0002703           39.50         0.2755         0.22544         0.0037965           40.03         0.1675         0.22544         0.0037967           40.51         0.1515         0.22545         0.0073744           42.57         0.135         0.21499         0.0013156           43.58         0.4760         0.20554         0.00739966           43.58         0.4760         0.20554         0.0032969           44.52         0.158         0.0026243         1.161           44.52         0.1580         0.0022643         1.161           44.52         0.1580         0.0022643         1.161           45.84         0.2765         0.025113         1.161           9.38         0.2765         0.011134         1.161           52.19         0.2765         0.0021134         1.161           52.19         0.2765         0.011134         1.161         1.161           52.19         0.2765         0.0211134         1.161         1.161           52.19         0.1675         0.15250         0.021134         1.161 <td></td> <td></td> <td>22.00</td> <td>0.1575</td> <td>0.207504</td> <td>0.00220337</td> <td></td> <td></td> <td></td> <td></td>			22.00	0.1575	0.207504	0.00220337				
16         0.316.01         0.247833         0.00021349           37.63         0.4740         0.2208140         0.000070134           9.53         0.2165         0.228144         0.00330027           4.005         0.11975         0.222423         0.0002516           4.215         0.3165         0.2214940         0.000402516           4.2415         0.3160         0.2202434         0.000313637           4.444         0.3160         0.2023506         1.4444           4.453         0.3160         0.013754         0.00023506           4.454         0.3160         0.013754         0.00023506           4.455         0.3160         0.013754         0.00023506           4.455         0.3160         0.167325         0.0001724           4.458         0.3909         0.0012734         1.4456           5.447         0.3160         0.167325         0.1134           5.448         0.3160         0.167325         0.000172           5.544         0.3160         0.167324         0.0002424           5.545         0.3160         0.167325         0.0002173           5.546         0.3160         0.167325         0.00021733			33.88	0.66/4	0.264590	0.009560/9				
14         9.76.1         0.0160         0.2289400         0.00087935           93.13         0.0160         0.228144         0.00136027           44.05         0.13160         0.228124         0.00131627           44.97         0.13160         0.228129         0.00042516           4.9.71         0.1185         0.21694         0.00131051           44.94         0.1168         0.208139         0.00045777           44.93         0.3160         0.228139         0.00173966           44.94         0.3166         0.19772         0.00359764           44.93         0.31845         0.0042516         1.116           44.93         0.318450         0.0042514         1.116           44.35         0.318450         0.0042514         1.116           51.40         0.22710         0.175288         0.0002102           51.41         0.2370         0.175288         0.002102           53.52         0.021673         1.113         1.114           54.33         0.022173         1.1374         0.00241231           54.30         0.014673         0.0022173         1.1374           54.30         0.015670         0.00201731			36.24	0.3160	0.247883	0.00421349				
10         0.3160         0.2320216         0.00379/05           395.00         0.1975         0.225244         0.0035731           44.6.6         0.1016         0.225243         0.001317141           44.5.7         0.1183         0.21973         0.001317141           44.5.8         0.3160         0.2025888         0.00131705           44.5.8         0.3160         0.2025896         0.00131705           44.5.8         0.3160         0.00137966         1.11         1.11           44.5.8         0.3160         0.00237966         1.11         1.11           44.5.8         0.3160         0.002424         1.11         1.11           51.44         0.20350         0.0026214         1.11         1.11           51.43         0.2750         0.177485         0.0021114         1.11         1.11           51.44         0.0030         0.115758         0.0021114         1.11         1.11         1.11           51.44         0.0030         0.11578         0.0021114         1.11         1.11         1.11           51.44         0.003141         1.11         0.114         1.11         1.11         1.11         1.11           51.41			37.63	0.4740	0.239040	0.00607013				
15         92.95         0.228144         0.0036027           40.05         0.11975         0.222423         0.00353671           42.15         0.3555         0.214940         0.0002516           42.15         0.3160         0.222423         0.003316077           43.48         0.0161360         7774         0.002516           43.48         0.3160         0.129754         0.0023566           44.52         0.3160         0.139323         0.0023566           44.83         0.2765         0.17738         0.00252666           44.93         0.2765         0.17788         0.00262421           44.93         0.2765         0.177288         0.0021702           53.84         0.3160         0.167325         0.002162           54.83         0.3160         0.167325         0.002162           53.84         0.3160         0.167325         0.0021673           54.83         0.3160         0.167325         0.0021673           55.84         0.3160         0.167340         0.0021673           55.84         0.3160         0.15746         0.00201733           64.19         0.17360         0.00204043           61.07         0.012			30.13	0.3160	0.230216	0.00387965				
16         0.0013802/1           44         0.55         0.0013802/1           44         0.55         0.03160         0.22223         0.00073161           42.97         0.0185         0.214904         0.0013163         0.0014161           42.97         0.0185         0.214904         0.0013163         0.0014161           44.83         0.1185         0.214904         0.0013163         0.0014161           44.83         0.0353         0.0002516         0.001739804         0.001739804           44.84         0.119703         0.00026214         0.001739804         0.001739804           44.85         0.118503         0.00026244         0.00171484         0.00026244           51.40         0.22765         0.117580         0.000210102         0.0017184           52.19         0.2770         0.01758         0.00210102         0.0017184           53.20         0.0216738         0.0017178         0.0021125         0.0017184           64.19         0.4493         0.0149491         0.0014949         0.0014949           65.20         0.041714         0.0023126         0.0114949         0.0114949           65.42         0.44184         0.014997         0.00023126			39.13	0.3100	0.230210	0.00387903				
440.03         0.0196         0.225243         0.0026573           44.54         0.0160         0.22423         0.00173141           42.15         0.0160         0.00402516           41.84         0.0160         0.00402516           42.84         0.0155         0.00184777           44.55         0.0355         0.0023506           44.58         0.3160         0.0197546           44.58         0.3160         0.0197546           44.58         0.3160         0.0197546           44.58         0.3160         0.0127218           44.58         0.21758         0.16736           45.89         0.3160         0.16732           51.49         0.2756         0.177388           0.3160         0.167312         0.0026502           53.20         0.012701         1.344           64.19         0.0126130         0.0021763           9.395         0.1173         0.0126401           64.30         0.15740         0.00250126           64.31         0.46672         0.0025126           64.32         0.41697         0.0012038           64.33         0.4284         0.146672           0.03284 <td></td> <td></td> <td>39.50</td> <td>0.2765</td> <td>0.228144</td> <td>0.00336027</td> <td></td> <td></td> <td></td> <td></td>			39.50	0.2765	0.228144	0.00336027				
14         0.3555         0.22423         0.00073141           42.15         0.3555         0.214490         0.0002516           43.44         0.3160         0.200450         0.00131361           43.45         0.3160         0.2004576         0.00131361           43.84         0.3160         0.200576         0.00132506           43.85         0.3160         0.1032506         0.1141           44.85         0.3455         0.13850         0.000224218           45.81         0.2755         0.177485         0.0025421           51.14         0.2755         0.177485         0.0025193           51.19         0.2756         0.15735         0.0025193           55.40         0.2765         0.15735         0.0021134           55.40         0.2765         0.15730         0.157316           66.31         0.4603         0.15730         0.15781           67.41         0.4767         0.0021731         1.444           64.19         0.15730         0.15497         0.0021731           64.19         0.4769         0.0021731         1.444           64.19         0.47697         0.0021731         1.444           64.19			40.03	0.1975	0.225245	0.00236573				
11         0.3155         0.214994         0.001313G1           42.97         0.1185         0.210490         0.001313G1           43.98         0.3160         0.208139         0.00345777           43.98         0.3160         0.11774         0.00132660           44.80         0.3160         0.11774         0.001325660           46.86         0.3260         0.01372661         1.0111           90.97         0.4345         0.01372660         1.0111           46.86         0.32760         0.115863         0.00072018         1.0111           90.97         0.4345         0.0187486         0.0002102         1.0111           51.49         0.2370         0.175268         0.002102         1.0111           53.64         0.3160         0.167325         0.002602         1.0111           53.64         0.3160         0.167325         0.002602         1.01114           64.75         0.158520         0.0026123         1.0111         1.01114           53.64         0.3160         0.0121731         1.01114         1.01114           64.75         0.012673         1.01114         1.01114         1.01114           64.75         0.012740			40.56	0.3160	0.222423	0.00373141				
14         24.77         0.1153         0.210940         0.00131363           43.88         0.4740         0.205818         0.00145477         0.00135764           44.52         0.5355         0.00378966         0.00137986         0.00137986           46.53         0.5355         0.00378961         0.001379861         0.001379861           46.54         0.3990         0.019233         0.00379861         0.0012014           40.54         0.3454         0.1189800         0.0042214         0.0012941           40.54         0.2370         0.168716         0.00201114         0.0012941           51.49         0.2370         0.168716         0.00201302         0.0011314           54.54         0.3100         0.168716         0.00201302         0.0011314           54.54         0.3100         0.168716         0.00201302         0.001141           64.35         0.01630         0.15326         0.00201301         0.0011411           64.36         0.014994         0.00046403         0.0011411         0.0031449           64.37         0.4030         0.151740         0.0030449         0.0031441           64.36         0.418994         0.00084493         0.0014141         0.001			42.15	0.3555	0.21/30/	0.00402516				
14         0.10         0.01014150           43.58         0.013159           43.58         0.0305         0.0037896           44.52         0.0355         0.0037896           44.58         0.9390         0.19923         0.0023266           47.66         0.04345         0.189691         0.0002221           47.66         0.4345         0.189691         0.002224           51.49         0.2755         0.188408         0.002224           51.49         0.2756         0.187160         0.00210131           54.38         0.2750         0.167325         0.0025602           55.44         0.3100         0.167325         0.00261233           55.45         0.3100         0.167325         0.00261233           55.40         0.3160         0.167325         0.00226123           55.41         0.3160         0.167325         0.00226123           64.35         0.46672         0.00231212			42.15	0.1105	0.214394	0.00402510				
143.88         0.160         0.208139         0.00143777           43.88         0.01700         0.208588         0.00171135           44.58         0.3530         0.200314         0.00179866           46.58         0.3540         0.203150         0.00179866           46.58         0.3540         0.189931         0.00137806           49.38         0.2765         0.184563         0.0020224           51.47         0.4345         0.180830         0.00002254           51.47         0.2775         0.0177485         0.00201102           54.57         0.02765         0.0177485         0.00201102           54.57         0.01760         0.0177485         0.00201102           54.57         0.01760         0.015601         0.0011778           59.40         0.156701         0.0011778         1.0001778           61.07         0.46672         0.0037612         1.01974           61.42         0.1730         0.14977         0.0013012           64.73         0.014677         0.0033014         1.01974           64.73         0.014677         0.0033014         1.019750           7.046         0.13570         0.00331313         1.014672			42.97	0.1185	0.210490	0.00131363				
143.98         0.47.90         0.205858         0.00512159           44.52         0.3555         0.03555         0.0375906           46.55         0.3556         0.039930         0.00732696           47.56         0.4343         0.189690         0.0002241           48.97         0.4343         0.189690         0.0002241           52.99         0.2770         0.177268         0.001201           54.38         0.2370         0.168716         0.00025692           54.44         0.3160         0.165716         0.00205692           54.45         0.3160         0.165716         0.00201702           54.38         0.2370         0.165726         0.00205692           54.44         0.3160         0.165910         0.00261293           54.47         0.3160         0.155910         0.00261293           64.39         0.41640         0.155901         0.00261293           64.39         0.416907         0.0032142         0.416917           64.39         0.416977         0.0032046         149977           64.39         0.416977         0.0032046         14977           70.08         0.5940         0.132760         0.0032046			43.48	0.3160	0.208139	0.00345777				
44.52         0.2535         0.203159         0.00273966           45.85         0.3600         0.199223         0.00397804           47.66         0.4345         0.188961         0.0026218           47.66         0.4345         0.188508         0.0020242           51.43         0.2763         0.177486         0.00210113           51.43         0.2764         0.177486         0.00210113           51.43         0.3100         0.167315         0.0026423           51.44         0.3100         0.167315         0.0026123           51.45         0.3100         0.167315         0.0026123           51.46         0.3160         0.167315         0.0026123           51.47         0.3100         0.159741         1.03954         1.395540           6.137         0.4033         0.151740         0.0024171         1.55641           6.137         0.4033         0.151740         0.0024171         1.55641           6.137         0.40397         0.002083         1.55744         1.395540           6.137         0.43697         0.002384         1.5576         1.5574           6.137         0.136970         0.0031246         1.557         1.5574			43.98	0.4740	0.205888	0.00512159				
14589         0.3100         0.197734         0.00325696           46.55         0.3950         0.199333         0.00397804           47.66         0.4345         0.189930         0.00326244           49.38         0.2765         0.189530         0.0056244           51.49         0.2775         0.189150         0.0026224           51.49         0.2775         0.175148         0.0001102           54.54         0.2170         0.175208         0.0001102           55.54         0.2170         0.175300         0.00211758           58.20         0.2765         0.15501         0.00211758           59.40         0.1610         0.155201         0.00211758           59.40         0.1600         0.155201         0.00211758           61.07         0.04692         1.49551-05         1.49551-05           61.07         0.04692         0.416972         0.00212125           64.34         0.17300         0.149070         0.0012035           64.35         0.93940         0.146972         0.0023483           64.36         0.3310         0.137460         0.0023484           7.099         0.5414         0.13806         0.0023044			44 52	0 3555	0.203515	0.00378966				
41.25         0.1919         0.1919         0.00397807           41.95         0.4345         0.0126324         1           41.94         0.2755         0.188901         0.002224           50.47         0.2370         0.168716         0.0022134           51.49         0.2755         0.173258         0.0025181           51.49         0.2765         0.173258         0.00251030           54.87         0.3160         0.163251         0.0026103           54.87         0.3160         0.163251         0.00261738           55.44         0.3160         0.153264         0.00211314           60.37         0.0030         0.00211731         1           61.07         0.4603         0.153944         0.00341731           62.32         0.94810         0.153944         0.00210238           61.07         0.4603         0.153944         0.00210238           64.75         0.4526         0.14970         0.00321312           63.32         0.51914         0.14970         0.0032143           64.75         0.24926         0.14970         0.0032143           7.46         0.5304         0.137866         0.0021216           7.76			45.90	0.2160	0.107754	0.00225606				
46.85         0.19990         0.19992         0.000472018           47.96         0.184631         0.000262218         1           47.96         0.2765         0.184630         0.000250181           51.91         0.2275         0.173258         0.00021012           51.91         0.2275         0.173258         0.0002102           51.84         0.3160         0.165125         0.00026123           55.45         0.3160         0.165120         0.0002173           55.40         0.3160         0.155940         1.49551-05           61.07         0.4603         0.1574740         0.000244731           63.32         0.49340         0.00144489         1.49551-05           61.17         0.4603         0.157740         0.00024492           63.42         0.46113         0.148951         0.4032           64.13         0.41810         0.149941         0.00024489           63.43         0.41870         0.000240312         1.49717           63.43         0.41870         0.00024084         1.49717           70.99         0.2581         0.13276         0.0013412           77.70         0.93805         0.13276         0.0013404 <tr< td=""><td></td><td></td><td>45.89</td><td>0.3160</td><td>0.19//34</td><td>0.00323696</td><td></td><td></td><td></td><td></td></tr<>			45.89	0.3160	0.19//34	0.00323696				
14         97.96         0.04345         0.084503         0.00062234           49.38         0.02765         0.0184503         0.00020234           51.49         0.27570         0.177485         0.00211134           54.38         0.02161         0.00211134           54.38         0.02161         0.0021102           54.27         0.16710         0.0021102           54.28         0.0216         0.16710         0.0021102           54.29         0.2765         0.017550         0.00214731           55.95         0.1075         0.15304         0.00149411           60.53         0.0022         0.15394         0.00240499           62.32         0.9480         0.145970         0.0023132           63.42         0.4480         0.149971         0.0032132           64.75         0.45620         0.0032132         0.44911           65.36         0.5994         0.142970         0.0032132           64.75         0.44560         0.00120588			46.85	0.3950	0.193923	0.00397804				
$16 \\ 40, 30 \\ 40, 3$			47.96	0.4345	0.189691	0.00426218				
50.47         0.4345         0.17485         0.00025181           51.49         0.2370         0.17485         0.0021134           54.38         0.3160         0.167325         0.00226123           55.64         0.3160         0.167325         0.00261293           58.20         0.2765         0.158501         0.00214731           60.33         0.015501         0.00214731         0.00214731           60.35         0.0020         0.15801         0.00214731           60.35         0.0202         0.15801         0.00214731           60.35         0.0202         0.15801         0.00214731           60.35         0.0202         0.15801         0.00214731           60.35         0.0220         0.15801         0.00214483           61.07         0.4603         0.151740         0.00240238           64.35         0.44826         0.418977         0.0032126           64.36         0.5094         0.414970         0.00314483           67.04         0.3050         0.137866         0.0013474           70.75         0.94810         0.126976         0.00324483           71.1         1.8         0.18460         0.0003474			49.38	0.2765	0.184563	0.00262424				
16         91.49         0.2785         0.17348         0.00031114           51.49         0.2370         0.167326         0.000211134           54.38         0.3160         0.167325         0.00025602           55.64         0.3160         0.167325         0.000210302           58.20         0.2765         0.15520         0.00021034           59.940         0.3160         0.15304         0.000214731           59.95         0.1975         0.15304         0.00034489           64.33         0.46622         0.00034489           64.34         0.416672         0.00034483           64.43         0.416672         0.00034483           64.74         0.13730         0.014921           65.36         0.5994         0.020388           64.75         0.43821         0.00324084           64.74         0.31976         0.00324984           74.90         0.52841         0.0132476           70.99         0.5281         0.0132476           72.32         0.9480         0.126310           73.76         0.0033791         0.147476           70.99         0.5341         0.132776         0.0033791           12.73 <td></td> <td></td> <td>50.47</td> <td>0.4345</td> <td>0 180830</td> <td>0.00402254</td> <td></td> <td></td> <td></td> <td></td>			50.47	0.4345	0 180830	0.00402254				
14.9         0.2183         0.017435         0.00211134           52.19         0.2370         0.167110         0.00211134           54.34         0.3160         0.167110         0.00211302           55.40         0.3160         0.15501         0.0021731           59.90         0.31560         0.0021731           60.33         0.0021         0.0021731           60.33         0.0020         0.015296           61.77         0.4603         0.015296           61.32         0.4403         0.0149411           62.32         0.9480         0.00064093           63.42         0.4403         0.145997           0.0120358         0.145997         0.0023131           65.36         0.5094         0.0120358           64.75         0.44256         0.143977         0.0034433           67.04         0.3505         0.0120381         0.167140           70.99         0.5541         0.12776         0.0035414           72.33         0.0480         0.126810         0.0053416           12.33         0.34612         0.0032465         1.1278           12.33         0.34510         0.0032464         1.1273			51.40	0.4345	0.180830	0.00402234				
16         52.19         0.2370         0.168716         0.00201302           54.87         0.3160         0.165735         0.00266402           55.8.40         0.3160         0.165191         0.00261293           58.40         0.3160         0.15561         0.00214731           60.35         0.002161731         0.00241731           60.35         0.0020         0.12964         1.4955405           61.47         0.4603         0.151740         0.00241731           62.32         0.9480         0.14607         0.003204           63.42         0.4461         0.14677         0.0032183           64.15         0.14610         0.14677         0.0033212           67.44         0.35661         0.0137476         0.0033214           67.44         0.35705         0.0139645         0.001344633           70.98         0.2788         0.137476         0.00497819           70.38         0.2788         0.126310         0.0003346           17.33         0.0381         0.0903794         0.003346           17.33         0.0384         0.0126190         0.003346           16.21         0.09384         0.039307         0.0003346			51.49	0.2765	0.1//485	0.00250181				
54.38         0.2370         0.167325         0.00265602           55.64         0.3160         0.167325         0.00261293           58.20         0.2765         0.03160         0.00216758           59.940         0.3160         0.155101         0.00214751           59.95         0.1975         0.019411         0.0154140           60.33         0.0020         0.1512400         0.0034489           62.32         0.9480         0.148970         0.0032165           64.47         0.414037         0.00320126         0.014941           64.32         0.4480         0.148977         0.0032182           67.04         0.43057         0.00320384         0.0149413           67.04         0.3505         0.139070         0.00320384           67.04         0.3505         0.0139476         0.003112           70.99         0.5544         0.03171         0.003114           71.76         0.44820         0.00324483           72.33         0.01371         0.065401           73.30         0.0331         0.003346           12.33         0.01371         0.648492           12.33         0.01370         0.003344			52.19	0.2370	0.175268	0.00211134				
16         \$4,87         0.3160         0.165191         0.00261293           58.20         0.2765         0.158501         0.00211731           59.93         0.1975         0.15304         0.00141411           60.33         0.0020         0.152964         1.49555-05           61.07         0.4603         0.115904         0.0016403           62.32         0.9480         0.146972         0.0005403           63.42         0.4618         0.146972         0.0013264           64.17         0.143977         0.00132132           65.36         0.5094         0.00134643           67.44         0.3305         0.13965         0.00134643           67.45         0.3305         0.13965         0.00134643           67.46         0.3305         0.13965         0.00134643           67.47         0.3305         0.13976         0.00134643           70.99         0.5541         0.12077         0.0033146           72.33         0.9480         0.12087         0.0032145           12.33         0.0371         0.0032466         1.217         0.2178           13.44         0.1275         0.033216         1.417         0.41843 <t< td=""><td></td><td></td><td>54.38</td><td>0.2370</td><td>0.168716</td><td>0.00201302</td><td></td><td></td><td></td><td></td></t<>			54.38	0.2370	0.168716	0.00201302				
16              5.5.4          0.1619          0.00216738            16              5.9.4          0.1360          0.158520          0.00216738            16              6.0.3          0.0120          0.0124711          0.00214731            17.0         0.4603          0.151740          0.0134419          0.0134419            16.1           0.0130          0.013449          0.0032165            16.4         0.14307          0.01320126          0.013449          0.0032165            16.4         0.14307          0.0032165          0.0032165          0.0032164            17.5           0.14397          0.0032164          0.0032164            17.7           0.13707          0.002388          0.002174463            17.8           0.13707          0.0003141          0.0007319            70.99            0.12610          0.0032645          0.003264            12.33            0.1371			54 87	0 3160	0 167325	0.00265602				
16         0.01619/1         0.00216758           16         0.0216         0.155520         0.00216758           16         0.020         0.155501         0.00216758           17         0.0430         0.0149411         0.00241731           59.95         0.1975         0.14304         0.0024449           61.23         0.0020         0.151740         0.00324489           62.32         0.9480         0.148971         0.00320125           64.12         0.143077         0.0032125         0.143077           64.75         0.4826         0.143977         0.0032142           67.06         0.5534         0.13976         0.0032142           67.06         0.5541         0.13976         0.0032988           68.06         0.27376         0.0033014         1           74.76         0.94860         0.126370         0.0033014           75.23         0.9480         0.126370         0.003246           12.93         0.1371         0.0653685         1         1           12.33         0.0381         0.269870         0.003246           12.33         0.0384         0.0053645         1           12.33         0.0381 <td></td> <td></td> <td>55.64</td> <td>0.3100</td> <td>0.107525</td> <td>0.00205002</td> <td></td> <td></td> <td></td> <td></td>			55.64	0.3100	0.107525	0.00205002				
58.20         0.2765         0.135820         0.00211731           59.99         0.1975         0.154344         0.00149411           60.33         0.0020         0.135266         1.49551-05           61.07         0.4603         0.115194         0.0034489           63.42         0.4618         0.146672         0.00328162           64.75         0.4626         0.143977         0.00323122           65.36         0.5904         0.143977         0.00323123           65.36         0.5904         0.143977         0.00332152           65.36         0.5904         0.13766         0.00097819           70.09         0.5541         0.13767         0.0033014           70.99         0.5541         0.12617         0.0033443           74.76         0.9480         0.126310         0.00034443           72.33         0.9480         0.126310         0.0032466           12.33         0.137         0.63630         0.0032466           12.33         0.137         0.636412         0.0022711           13.84         0.1755         0.53970         0.00304663           12.37         0.30804         0.0093978           18.31 <td< td=""><td></td><td></td><td>55.64</td><td>0.3160</td><td>0.165191</td><td>0.00261293</td><td></td><td></td><td></td><td></td></td<>			55.64	0.3160	0.165191	0.00261293				
59.40         0.31600         0.015801         0.00214731           59.59         0.1975         0.135340         0.00149411           60.53         0.0020         0.132964         1.43551-05           61.07         0.4603         0.00340489         0.0064083           63.42         0.4618         0.146677         0.0022058           64.175         0.4826         0.143977         0.00320126           64.19         0.1730         0.144997         0.00320844           65.36         0.5904         0.142780         0.00346483           67.04         0.3505         0.0023084           66.00         0.131760         0.000397819           70.08         0.2778         0.132670         0.0013406           72.33         0.9480         0.126987         0.0033466           12.73         0.0480         0.126987         0.0033466           12.73         0.0481         0.0033686			58.20	0.2765	0.158520	0.00216758				
59.95         0.1975         0.14304         0.00149411           60.33         0.0020         0.132964         1.49551-05           61.07         0.4603         0.131740         0.00340489           63.42         0.4618         0.146974         0.0032122           64.19         0.1700         0.01323122         64618         0.146974           64.175         0.4826         0.132977         0.00321322           64.04         0.35064         0.142977         0.0032182           67.04         0.3506         0.0203884         0.00146483           66.06         0.131906         0.00097819         0.00174476           70.08         0.2788         0.132072         0.00174476           71.76         0.9480         0.126070         0.0033014           74.77         0.9480         0.126070         0.0033046           72.33         0.0483         0.040610         0.00037846           12.33         0.0183         0.050430         0.00037978           16.37         0.3098         0.54612         0.0023095           16.37         0.3098         0.54612         0.0023793           16.37         0.3180         0.00146394         0.97751			59.40	0.3160	0.155601	0.00241731				
16         0.0020         0.152964         1.4958:0.5           16         0.033         0.0020         0.151740         0.00340499           16.2.32         0.9480         0.145977         0.00120358           16.4.19         0.1770         0.145977         0.00120358           16.4.25         0.4266         0.143977         0.0032122           16.5.56         0.3904         0.132860         0.00346483           16.7.74         0.35174         0.00339014         1.5776           17.700         0.137866         0.00138698         1.5776           17.700         0.27818         0.13176         0.00139014           70.09         0.5541         0.132776         0.0033014           71.75         0.9480         0.1320776         0.00330436           71.75         0.39401         0.12777         0.00331414           72.73         0.0451         0.00374144         1.273           71.75         0.35310         0.0053046         1.273           13.84         0.1755         0.53970         0.0030946           12.73         0.3614         0.0028795         1.573           13.81         0.2765         0.3939377         0.00454635 <td></td> <td></td> <td>59.95</td> <td>0 1975</td> <td>0 154304</td> <td>0.00149411</td> <td></td> <td></td> <td></td> <td></td>			59.95	0 1975	0 154304	0.00149411				
16         0.0023         0.01294         1.12304           61.07         0.4030         0.01148994         0.00084083           62.32         0.9480         0.148994         0.00084083           63.42         0.418097         0.00021256           64.19         0.1730         0.145097         0.00021256           64.75         0.48220         0.143170         0.0034043           65.36         0.5094         0.142780         0.0034043           66.00         0.313         0.136700         0.0032084           66.00         0.2917         0.137866         0.00023084           68.66         0.15317         0.40278         0.0132016           70.98         0.2788         0.134275         0.000173476           70.99         0.5541         0.13276         0.0033014           74.76         0.9480         0.126370         0.00323014           74.76         0.9480         0.126370         0.00323785           11.58         0.1816         0.764192         0.00273785           12.31         0.2216         0.033384         0.01061622           12.31         0.216         0.338017         0.00614233           22.80			60.52	0.0020	0.152064	1 4055E 05				
61.07         0.4403         0.131740         0.00340489           63.32         0.9480         0.148672         0.00326126           64.19         0.1730         0.145077         0.0032312           65.36         0.5994         0.143977         0.0032132           65.36         0.5994         0.142700         0.0012038           67.04         0.3505         0.139605         0.00230844           68.06         0.131         0.136701         0.00097819           70.99         0.5541         0.13276         0.0033014           74.6         0.9480         0.126808         0.01268698           68.66         0.12610         0.00078140         0.0033014           75.23         0.9480         0.126310         0.00032466           12.93         0.1371         0.684692         0.00032466           12.93         0.1371         0.684692         0.00032466           15.73         0.038         0.545163         0.00039798           16.37         0.3908         0.545482         0.00037978           16.37         0.39083         0.440433         0.0156638           20.71         0.1860         0.428902         0.00032015			60.33	0.0020	0.152964	1.4955E-05				
62.32         0.9480         0.148994         0.00064083           63.42         0.4418         0.145097         0.00120358           64.75         0.44250         0.143707         0.00031212           65.36         0.5094         0.142780         0.00034643           67.70         0.0305         0.00030844           68.00         0.2917         0.13786         0.00188084           68.66         0.1531         0.13610         0.000797819           70.09         0.5541         0.132776         0.0033014           74.76         0.9480         0.126310         0.00037464           73.23         0.9480         0.126310         0.0003746           11.38         0.1317         0.603034         0.0003446           12.73         0.0363         0.695403         0.0003746           13.84         0.1755         0.639870         0.00039798           16.37         0.3090         0.544513         0.00639798           16.37         0.3090         0.45453         0.0064623           22.80         0.0675         0.339037         0.0044159           22.74         0.37604         0.390037         0.0044523           23.60			61.07	0.4603	0.151740	0.00340489				
63.42         0.4618         0.146072         0.00326126           64.19         0.17300         0.143997         0.00332132           65.36         0.5944         0.142780         0.00332132           65.36         0.5944         0.142780         0.00332132           65.36         0.5944         0.139660         0.00320884           68.00         0.2917         0.137866         0.00078149           70.99         0.5541         0.13275         0.00079719           70.99         0.5541         0.13276         0.00039014           74.76         0.9480         0.126987         0.00051414           73.3         0.9480         0.126987         0.000539146           12.73         0.0083         0.695403         0.000527911           13.84         0.1755         0.69870         0.00053976           15.37         0.3361         0.56388         0.01061622           16.31         0.0938         0.54150         0.00939798           18.31         0.2215         0.373871         0.00563946           23.04         0.1850         0.37061         0.09039354           23.05         0.1275         0.373871         0.00263955			62.32	0.9480	0.148994	0.00684083				
16         10,1730         0.145007         0.00120358           64,75         0.4426         0.00321132         0.00324443           65,36         0.5094         0.142780         0.00324643           67,04         0.3505         0.0023084         0.0023084           68,66         0.1531         0.13706         0.00097819           70.99         0.5541         0.013275         0.00173476           70.99         0.5541         0.0032017476         0.0033014           74.76         0.9480         0.126310         0.00350836           12,73         0.0933         0.695403         0.00032466           12,73         0.0331         0.6639870         0.00032466           12,73         0.0331         0.6639870         0.00032057911           13,84         0.0126         0.0037791         0.003309364           16,21         0.0338         0.54383         0.00046638           20,71         0.1860         0.428902         0.0043663           21,280         0.175         0.33787         0.00046638           22,80         0.0673         0.390037         0.00146585           22,80         0.0673         0.390041         0.0024734			63 42	0 4618	0 146672	0.00326126				
16         -0.130         0.14307         0.00120338           65.36         0.5094         0.142780         0.0034483           65.36         0.5094         0.142780         0.0033014           65.36         0.5094         0.142775         0.0033014           68.00         0.2917         0.137866         0.00188698           68.66         0.1511         0.136776         0.00039014           70.99         0.5541         0.013776         0.0033014           74.76         0.9480         0.126987         0.00341414           72.32         0.9490         0.126987         0.00339014           12.73         0.00480         0.126987         0.00339016           12.73         0.00480         0.00033946         0.00032466           12.73         0.00480         0.00039798         0.00039798           15.73         0.331         0.0039798         0.00039798           16.21         0.0938         0.546812         0.00287395           22.58         0.2765         0.373871         0.0024658           23.60         0.1255         0.370941         0.002473           24.05         0.1450         0.36022         0.00444159			64.10	0.1720	0.145007	0.00120259				
64.75         0.4826         0.0143977         0.000332132           67.04         0.3505         0.139605         0.00230884           67.04         0.3505         0.139705         0.0007819           70.08         0.2788         0.134775         0.00178476           70.99         0.5541         0.132776         0.00330014           71.76         0.9480         0.126310         0.000336836           72.32         0.9480         0.126310         0.0033046           72.33         0.0383         0.64902         0.00032466           12.93         0.13171         0.684692         0.00032466           12.93         0.1315         0.639870         0.00030946           15.73         0.3361         0.563388         0.01061622           16.21         0.0938         0.541503         0.0093795           22.58         0.2755         0.037307         0.0044635           22.54         0.2757         0.037377         0.0044635           22.54         0.2757         0.337377         0.0044635           22.54         0.2757         0.339024         0.0045640           22.55         0.27570         0.339024         0.0024754			04.19	0.1730	0.143097	0.00120338				
65.36         0.5094         0.142780         0.00346483           67.04         0.3505         0.137866         0.00188698           68.66         0.5131         0.137610         0.00097819           70.98         0.2788         0.134275         0.00138608           70.99         0.5541         0.13276         0.0033014           71.76         0.9480         0.126310         0.00356836           71.77         0.9480         0.126310         0.00356836           71.78         0.04816         0.76192         0.00781440           72.73         0.0383         0.6684692         0.00527911           71.84         0.1755         0.639870         0.00630946           71.75         0.3361         0.563388         0.01061622           71.81         0.219         0.434533         0.00546638           72.78         0.2756         0.339787         0.00604923           72.81         0.2756         0.339787         0.00604923           72.81         0.2756         0.339787         0.00604923           72.81         0.1860         0.345061         0.0039054           72.81         0.1860         0.345061         0.0039054			64.75	0.4826	0.143977	0.00332132				
67.04         0.3505         0.0139665         0.00230884           68.00         0.2278         0.135766         0.00188698           68.66         0.1531         0.136701         0.00097819           70.08         0.2788         0.134275         0.00133014           74.76         0.9480         0.126987         0.0033014           74.76         0.9480         0.126097         0.0033044           72.33         0.9480         0.1260987         0.0033266           12.93         0.1371         0.684692         0.0033246           12.93         0.1375         0.63388         0.01061622           15.73         0.3361         0.563388         0.01061622           16.21         0.039         0.346812         0.0039078           18.31         0.2109         0.484543         0.0039054           22.58         0.2765         0.39377         0.00416535           23.04         0.1836         0.386028         0.0032045           24.30         0.1836         0.36040         0.977514         1.046536         11.3         NA           16         corrystal         25.82         0.0799         0.0042635         2380         1.13         N			65.36	0.5094	0.142780	0.00346483				
68.00         0.2917         0.137866         0.00188698           68.66         0.1331         0.136701         0.0097819           70.99         0.5541         0.132776         0.00330014           74.76         0.9480         0.126987         0.0033014           75.23         0.9480         0.126987         0.00336836           11.58         0.1816         0.76492         0.00737846           12.93         0.083         0.695403         0.00032466           12.93         0.1371         0.684692         0.0032466           15.73         0.3361         0.563388         0.01061622           16.37         0.3998         0.54453         0.00032791           18.31         0.21019         0.484543         0.00287395           16.37         0.3908         0.34453         0.0039064           22.58         0.2765         0.33977         0.000404159           22.58         0.2765         0.33977         0.00060432           23.60         0.0322         0.37694         0.001945635           23.60         0.1350         0.360290         0.00242734           24.30         0.1580         0.360290         0.002248973			67.04	0 3505	0 139605	0.00230884				
68.00         0.231         0.137400         0.00097819           70.08         0.2788         0.134275         0.00097819           70.08         0.2788         0.012976         0.00039014           74.76         0.9480         0.120987         0.00514141           75.3         0.9480         0.12087         0.00336836           11.58         0.1816         0.764192         0.00781440           12.73         0.0083         0.695403         0.00032466           15.73         0.03361         0.563388         0.01061622           16.31         0.2019         0.484543         0.00039798           18.31         0.2019         0.484543         0.00046638           20.71         0.1860         0.428902         0.0024739           22.80         0.675         0.399037         0.00046323           22.80         0.675         0.399037         0.00046638           23.40         0.1880         0.366280         0.00320215           24.30         0.1880         0.366290         0.0032265           24.30         0.180         0.366290         0.00322345           24.30         0.180         0.366290         0.000322454			68.00	0.2017	0.127866	0.00250001				
68.86         0.1331         0.136701         0.00097819           70.99         0.5541         0.132776         0.00339014           74.76         0.99480         0.12697         0.00034144           75.23         0.9480         0.12697         0.00032466           12.93         0.1371         0.684692         0.0002781440           12.73         0.0083         0.695403         0.00032466           12.93         0.1371         0.684692         0.000227911           13.84         0.1755         0.633870         0.0003946           15.73         0.3361         0.563388         0.01061622           16.21         0.0938         0.546812         0.00287395           18.31         0.219         0.484543         0.00346638           22.58         0.2765         0.393787         0.00049233           23.60         0.0332         0.6673         0.390037           23.60         0.1386         0.386028         0.0039215           24.05         0.1185         0.370941         0.0045639           23.04         0.1806         0.46290         0.0032015           24.05         0.1185         0.370941         0.0045639			08.00	0.2917	0.15/800	0.00188098				
70.08         0.2788         0.134275         0.000739014           74.76         0.9480         0.126987         0.000339014           74.76         0.9480         0.126987         0.000339014           72.32         0.9480         0.126987         0.000781440           12.73         0.0083         0.695403         0.00032466           12.93         0.1371         0.684692         0.00630946           15.73         0.3361         0.563388         0.01061622           16.21         0.0938         0.546112         0.00287395           16.37         0.3098         0.544513         0.00034663           20.71         0.1860         0.428902         0.00444159           22.58         0.2765         0.3393787         0.00604323           23.04         0.1836         0.366020         0.0032015           23.40         0.1850         0.366290         0.00230215           23.40         0.1275         0.378871         0.00263945           24.05         0.1185         0.370411         0.00230215           23.40         0.1275         0.373871         0.0022473           24.05         0.1185         0.370341         0.0022473			68.66	0.1531	0.136701	0.00097819				
70.99         0.5541         0.132776         0.00339014           74.76         0.9480         0.126310         0.00536836           11.58         0.1816         0.764192         0.00781440           12.73         0.0383         0.659403         0.00032466           12.93         0.1371         0.684692         0.006297911           13.84         0.1755         0.639870         0.00630946           15.73         0.3616         0.56338         0.01061622           16.21         0.0938         0.544812         0.00287395           18.31         0.2019         0.484543         0.0054632           22.58         0.2765         0.393787         0.0064323           22.80         0.0673         0.338002         0.0032605           23.60         0.1275         0.37871         0.00263995           24.05         0.1185         0.370041         0.0024734           23.60         0.1275         0.373871         0.0026394           24.05         0.1185         0.370041         0.0022473           24.05         0.1185         0.370041         0.0022473           24.05         0.1185         0.338024         0.977514         1.046536 <td></td> <td></td> <td>70.08</td> <td>0.2788</td> <td>0.134275</td> <td>0.00173476</td> <td></td> <td></td> <td></td> <td></td>			70.08	0.2788	0.134275	0.00173476				
Monomer         25.2         0.3480         0.126987         0.00341414           75.23         0.9480         0.126310         0.00356836           11.58         0.1816         0.764192         0.000781440           12.73         0.0083         0.695403         0.00032466           12.93         0.1371         0.684692         0.00527911           13.44         0.1755         0.639870         0.00032936           16.21         0.0938         0.546122         0.0023795           16.37         0.3098         0.541503         0.0093798           18.31         0.2019         0.484533         0.00546638           22.88         0.0765         0.39037         0.0004323           23.80         0.1275         0.370941         0.0023015           23.80         0.1275         0.373871         0.00263955           24.05         0.11880         0.366290         0.0033021           24.30         0.1580         0.366290         0.00230215           23.80         0.1275         0.373871         0.0024273           24.05         0.1184         0.310210         0.0024273           24.30         0.1580         0.366290         0.00320215 </td <td></td> <td></td> <td>70.99</td> <td>0 5541</td> <td>0 132776</td> <td>0.00339014</td> <td></td> <td></td> <td></td> <td></td>			70.99	0 5541	0 132776	0.00339014				
14.1.0         0.9480         0.12857         0.00341414           75.23         0.9480         0.126310         0.00336836           11.58         0.1816         0.764192         0.0032466           12.73         0.0083         0.695403         0.00032466           12.93         0.1371         0.684692         0.000327911           13.84         0.1755         0.639870         0.00030946           15.73         0.3361         0.563388         0.01061622           16.21         0.0938         0.54812         0.0023795           16.37         0.3098         0.541503         0.00039978           20.71         0.1860         0.428902         0.004414159           22.58         0.2755         0.339787         0.0064323           23.60         0.0932         0.376994         0.00324653           23.60         0.0932         0.376994         0.00242734           24.05         0.1185         0.376994         0.00242734           24.05         0.1850         0.366290         0.00320415           23.60         0.2794         0.278497         0.0042344           16         cocrystal         25.82         0.0790         0.033040 <td></td> <td></td> <td>70.77</td> <td>0.03941</td> <td>0.132770</td> <td>0.00537014</td> <td></td> <td></td> <td></td> <td></td>			70.77	0.03941	0.132770	0.00537014				
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$			/4./6	0.9480	0.126987	0.00541414				
11.58         0.1816         0.764192         0.00731440           12.73         0.0083         0.695403         0.00032466           12.93         0.1371         0.684692         0.00527911           13.84         0.1755         0.639870         0.00030946           15.73         0.3361         0.563388         0.01061622           16.21         0.0938         0.54812         0.0023795           16.37         0.3098         0.541503         0.000399788           20.71         0.1860         0.428902         0.00444159           22.58         0.2775         0.339787         0.0064323           23.60         0.0673         0.390037         0.00194658           23.60         0.0322         0.376994         0.00242734           24.05         0.1185         0.370041         0.00242734           24.05         0.1850         0.366290         0.0032015           23.60         0.2704         0.270490         0.00242734           24.05         0.1840         0.30304         0.097514         1.046536         11.3         NA           16         cocrystal         25.82         0.27070         0.349049         0.0022473         0.444			75.23	0.9480	0.126310	0.00536836				
Monomer         25.8         0.03700         0.0382466           12.93         0.1371         0.684692         0.00527911           13.84         0.1755         0.639870         0.00630946           15.73         0.3361         0.639870         0.00839946           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         0.0428902         0.00441159           22.58         0.2765         0.330787         0.0064323           23.04         0.1755         0.37694         0.00194563           23.80         0.1275         0.373871         0.00263995           24.05         0.1185         0.376094         0.00194654           23.80         0.1275         0.373871         0.00263995           24.05         0.1185         0.370041         0.0022734           24.05         0.1185         0.370441         0.00248973           24.05         0.1185         0.370441         0.0022473           30.94         0.2089         0.289029         0.00323044			11.58	0.1816	0 764192	0.00781440				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			12.72	0.0092	0.605402	0.00022466				
			12.75	0.0085	0.093403	0.00032400				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			12.93	0.1371	0.684692	0.0052/911				
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       0.00644159         22.58       0.2765       0.393787       0.00604323         22.80       0.0673       0.390037       0.00145635         23.04       0.1836       0.336028       0.0039054         23.60       0.1275       0.373871       0.00263995         24.05       0.1185       0.370694       0.00194658         23.80       0.1275       0.373971       0.00263995         24.05       0.1185       0.366290       0.00320215         24.05       0.1340       0.0015084       0.977514       1.046536       11.3       NA         (4-7)       28.78       0.1464       0.310210       0.0022473       3       3.61       0.2704       0.274599       0.00403344         33.65       0.2919       0.266346       0.00150384       0.977514       1.046536       11.3       NA         16       corrystal       25.82			13.84	0.1755	0.639870	0.00630946				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			15.73	0.3361	0.563388	0.01061622				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			16.21	0.0938	0.546812	0.00287395				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			16.21	0.0750	0.541502	0.00207595				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			10.57	0.3098	0.341303	0.00939/98				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			18.31	0.2019	0.484543	0.00546638				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			20.71	0.1860	0.428902	0.00444159				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			22.58	0.2765	0.393787	0.00604323				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			22.80	0.0673	0.300037	0.00145635				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			22.00	0.0075	0.370037	0.00145055				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			23.04	0.1836	0.386028	0.00393054				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			23.60	0.0932	0.376994	0.00194658				
$\begin{array}{c cccc} 24.05 & 0.1185 & 0.370041 & 0.00242734 \\ 24.30 & 0.1580 & 0.366290 & 0.00320215 \\ \hline Monomer & 25.52 & 0.2370 & 0.349049 & 0.00456640 \\ 16 & cocrystal & 25.82 & 0.0790 & 0.345061 & 0.00150384 & 0.977514 & 1.046536 & 11.3 & NA \\ \hline (4.7) & 28.78 & 0.1464 & 0.310210 & 0.00224873 \\ & 29.45 & 0.1340 & 0.303304 & 0.00222473 \\ & 30.94 & 0.2089 & 0.289029 & 0.00329345 \\ & 32.61 & 0.2704 & 0.274599 & 0.00403344 \\ & 33.65 & 0.2919 & 0.266346 & 0.00421190 \\ & 34.39 & 0.1019 & 0.260782 & 0.00143679 \\ & 34.51 & 0.2648 & 0.25903 & 0.00371988 \\ & 34.75 & 0.1205 & 0.258163 & 0.00168034 \\ & 34.93 & 0.1816 & 0.256874 & 0.00251847 \\ & 35.24 & 0.3160 & 0.254685 & 0.00434130 \\ & 36.74 & 0.1355 & 0.244624 & 0.00178042 \\ & 37.00 & 0.1442 & 0.242964 & 0.0018045 \\ & 38.76 & 0.1056 & 0.232328 & 0.00130988 \\ & 38.94 & 0.1814 & 0.231295 & 0.00223887 \\ & 41.20 & 0.1797 & 0.219115 & 0.0028604 \\ & 41.48 & 0.0007 & 0.217700 & 8.06E-060 \\ & 41.48 & 0.00890 & 0.21599 & 0.00101615 \\ \end{array}$			23.80	0.1275	0.373871	0.00263995				
$\begin{array}{c cccc} & 24.30 & 0.1580 & 0.366290 & 0.00320215 \\ \hline Monomer & 25.52 & 0.2370 & 0.349049 & 0.00456640 \\ 16 & cocrystal & 25.82 & 0.0790 & 0.345061 & 0.00150384 & 0.977514 & 1.046536 & 11.3 & NA \\ \hline (4.7) & 28.78 & 0.1464 & 0.310210 & 0.00248973 \\ & 29.45 & 0.1340 & 0.303304 & 0.00222473 \\ & 30.94 & 0.2089 & 0.289029 & 0.00329345 \\ & 32.61 & 0.2704 & 0.274599 & 0.00403344 \\ & 33.65 & 0.2919 & 0.266346 & 0.00421190 \\ & 34.39 & 0.1019 & 0.260782 & 0.0014679 \\ & 34.51 & 0.2648 & 0.259903 & 0.00371988 \\ & 34.75 & 0.1205 & 0.258163 & 0.00168034 \\ & 34.93 & 0.1816 & 0.256874 & 0.00251847 \\ & 35.24 & 0.3160 & 0.254685 & 0.00434130 \\ & 36.74 & 0.1355 & 0.244624 & 0.00188045 \\ & 37.00 & 0.1442 & 0.2242964 & 0.00188045 \\ & 38.76 & 0.1056 & 0.232328 & 0.00130988 \\ & 38.94 & 0.1814 & 0.231295 & 0.00223887 \\ & 41.20 & 0.1797 & 0.219115 & 0.0028604 \\ & 41.48 & 0.0007 & 0.217700 & 8.066E-060 \\ & 41.48 & 0.00890 & 0.215959 & 0.00101615 \\ \end{array}$			24.05	0 1185	0.370041	0.00242734				
$\begin{array}{c cccc} Monomer & 25.52 & 0.2370 & 0.349049 & 0.00456640 \\ 16 & cocrystal & 25.82 & 0.0790 & 0.345061 & 0.00150384 & 0.977514 & 1.046536 & 11.3 & NA \\ \hline (4.7) & 28.78 & 0.1464 & 0.310210 & 0.00248973 \\ & 29.45 & 0.1340 & 0.303304 & 0.00222473 \\ & 30.94 & 0.2089 & 0.289029 & 0.00329345 \\ & 32.61 & 0.2704 & 0.274599 & 0.00403344 \\ & 33.65 & 0.2919 & 0.266346 & 0.00421190 \\ & 34.39 & 0.1019 & 0.260782 & 0.00143679 \\ & 34.51 & 0.2648 & 0.259903 & 0.00371988 \\ & 34.75 & 0.1205 & 0.258163 & 0.00148054 \\ & 34.93 & 0.1816 & 0.256874 & 0.00251847 \\ & 35.24 & 0.3160 & 0.254685 & 0.0043140 \\ & 36.74 & 0.1355 & 0.244624 & 0.00178042 \\ & 37.00 & 0.1442 & 0.242964 & 0.00188045 \\ & 38.76 & 0.1056 & 0.232328 & 0.00130988 \\ & 38.94 & 0.1814 & 0.231295 & 0.00223887 \\ & 41.20 & 0.1797 & 0.219115 & 0.0028604 \\ & 41.48 & 0.0007 & 0.217700 & 8.066E-060 \\ & 41.48 & 0.00890 & 0.215959 & 0.00101615 \\ \end{array}$			24.20	0.1590	0.266200	0.00212751				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			24.30	0.1380	0.306290	0.00320213				
$\begin{array}{c cccc} 16 & cocrystal & 25.82 & 0.0790 & 0.345061 & 0.00150384 & 0.977514 & 1.046536 & 11.3 & NA \\ \hline (4.7) & 28.78 & 0.1464 & 0.310210 & 0.00248973 \\ & 29.45 & 0.1340 & 0.303304 & 0.00222473 \\ & 30.94 & 0.2089 & 0.289029 & 0.00329345 \\ & 32.61 & 0.2704 & 0.274599 & 0.00403344 \\ & 33.65 & 0.2919 & 0.266346 & 0.00421190 \\ & 34.39 & 0.1019 & 0.260782 & 0.00143679 \\ & 34.51 & 0.2648 & 0.259903 & 0.00371988 \\ & 34.75 & 0.1205 & 0.258163 & 0.00168034 \\ & 34.93 & 0.1816 & 0.256874 & 0.00251847 \\ & 35.24 & 0.3160 & 0.254685 & 0.0043130 \\ & 36.74 & 0.1355 & 0.244624 & 0.00178042 \\ & 37.00 & 0.1442 & 0.242964 & 0.00188045 \\ & 38.76 & 0.1056 & 0.232328 & 0.00130988 \\ & 38.94 & 0.1814 & 0.231295 & 0.00223887 \\ & 41.20 & 0.1797 & 0.219115 & 0.00208604 \\ & 41.48 & 0.0007 & 0.217700 & 8.066E-060 \\ & 41.83 & 0.0890 & 0.215959 & 0.00101615 \\ \end{array}$		Monomer	25.52	0.2370	0.349049	0.00456640				
	16	cocrystal	25.82	0.0790	0.345061	0.00150384	0.977514	1.046536	11.3	NA
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		(4.7)	28.78	0.1464	0.310210	0.00248973				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		(• ')	29.45	0 1340	0 303304	0.00222473				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			20.04	0.1040	0.200204	0.002224/3				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			30.94	0.2089	0.289029	0.00329345				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			32.61	0.2704	0.274599	0.00403344				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			33.65	0.2919	0.266346	0.00421190				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			34 39	0.1019	0.260782	0.00143679				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			24 51	0.1017	0.250002	0.00271000				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			34.51	0.2648	0.259903	0.003/1988				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			34.75	0.1205	0.258163	0.00168034				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			34.93	0.1816	0.256874	0.00251847				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			35 24	0.3160	0.254685	0.00434130				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			26 74	0.1255	0.237003	0.00170040				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$			30./4	0.1355	0.244624	0.001/8042				
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$			37.00	0.1442	0.242964	0.00188045				
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$			38.76	0.1056	0.232328	0.00130988				
41.20 0.1797 0.21915 0.00228604 41.48 0.0007 0.217700 8.066E-060 41.83 0.0890 0.215959 0.00101615			38 0/	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 20	0.1014	0.231273	0.00223007				
41.48 0.0007 0.217700 8.066E-060 41.83 0.0890 0.215959 0.00101615			41.20	0.1797	0.219115	0.00208604				
41.83 0.0890 0.215959 0.00101615			41.48	0.0007	0.217700	8.066E-060				
······································			41.83	0.0890	0.215959	0.00101615				

		41.07	0.0762	0 215271	0.00086707				
		41.97	0.0703	0.2132/1	0.00080797				
		43.43	0.0790	0.208367	0.00086554				
		44.17	0.1580	0.205046	0.00169908				
		45 50	0.1185	0 199357	0.00123303				
		45.50	0.1105	0.105300	0.00120305				
		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	0.2192	0.174420	0.00102221				
		32.40	0.2185	0.1/4430	0.00193321				
		53.00	0.1555	0.172779	0.00136085				
		54.93	0.0785	0.167157	0.00065896				
		55.62	0.1127	0.165218	0.00002200				
		55.05	0.1127	0.105218	0.00093209				
		55.79	0.1643	0.164/82	0.00135426				
		57.11	0.1857	0.161283	0.00148892				
		59.61	0.1962	0.155103	0.00149450				
		50.79	0.2028	0.154702	0.00152049				
		39.78	0.2028	0.134702	0.00133948				
		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	0.120220	0.00141459				
		07.25	0.2130	0.139220	0.00141438				
		72.36	0.1090	0.130596	0.00065030				
		72.61	0.1813	0.130207	0.00107672				
		73 42	0.0790	0 128970	0.00046229				
		75.42	0.0790	0.126970	0.00040227				
		/5.6/	0.1309	0.125685	0.000/3541				
		75.87	0.1115	0.125403	0.00062416				
		76.58	0.2078	0.124417	0.00114849				
		79 57	0.1625	0.120476	0.00085147				
		17.51	0.1023	0.1207/0	0.0000014/				
		11.05	0.4549	0.800723	0.02051987				
		11.24	0.5510	0.787230	0.02443202				
		12 30	0.4040	0.719616	0.01635964				
		12.50	0.1000	0.719010	0.010555704				
		15./4	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				
		10.07	0.1104	0.470288	0.00517720				
		18.8/	0.2302	0.4/0288	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	0.1010	0.441561	0.00250750				
		20.11	0.1017	0.42(400	0.00230730				
		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				
		21.50	0.0255	0.410675	0.00033050				
		21.04	0.2765	0.4106/3	0.00031231				
		21.89	0.2765	0.406041	0.00623866				
		22.21	0.2765	0.400263	0.00614653				
		22.51	0.2765	0.394996	0.00606251				
		22.22	0.1703	0.282076	0.00361677				
		23.22	0.1703	0.383070	0.003010/7				
		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				
		25.00	0.1102	0.34/1//	0.00220437				
	Monomer	25.89	0.0735	0.344144	0.00139523				
17	coornistal	26.74	0.1713	0.333395	0.00314472	0.077024	1 047564	8.0	NIA
1 /	cocrystar	26.89	0.1212	0.331569	0.00221211	0.977034	1.047304	8.0	INA
	(5.7)	27.16	0.1011	0 328334	0.00182621				
		28.04	0.2146	0.218226	0.00274000				
		20.04	0.2140	0.316220	0.003/4777				
		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				
		21 = 1	0.1090	0.200755	0.00421140				
		31.31	0.4081	0.283929	0.00031108				
		32.18	0.2765	0.278169	0.00418261				
		32.70	0.2765	0.273863	0.00411244				
		33.14	0.1451	0.270327	0.00212782				
		22.55	0.1120	0.267117	0.00163566				
		33.33	0.1130	0.20/11/	0.00105500				
		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				
		27 17	0.0012	0.244047	1 5/200 05				
		5/.4/	0.0012	0.240024	1.3438E-03				
		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				
		10.00	0.1717	0.227975	0.00202212				
		40.04	0.1/1/	0.222004	0.00202515				
		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				
		+2.//	0.17/3	0.170244	0.0020413.				

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

<sup>a</sup> The peak position (2 $\theta$ ) and full-width-of-half-maximum (FWHM) are generated from PXRD spectra and Match! software. <sup>b</sup> The d<sub>hkl</sub> spacing values are calculated from equation (3). <sup>c</sup> The microstrain (*c*) values are calculated from equation (4). <sup>d</sup> The crystallite sizes are calculated from equations (1) and (2) and the intercept values from Fig. S7. <sup>e</sup> The dislocation densities are calculated from equation (5). <sup>f</sup> *R*p is the R factor in Rietveld refinement, showing the discrepancy index between the experimental and calculated spectra. Normally, *R*<sub>p</sub> less than 10% indicates a good fit. <sup>s</sup> Match ratio (%) = (the number of peaks of the polymer identically matched with those of the monomer (red))  $\Sigma$  {(the number of peaks of 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)) × 100%. The matching ratio was calculated in pairs (entries 10 vs 11 and entries 13 vs 14).

# 7. *I*<sub>405</sub> and *I*<sub>488</sub> values

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

Entry	Mode <sup>a</sup>	Sample <sup>b</sup>	<i>I</i> <sub>405</sub> (a.u.) <sup>c</sup>	<i>I</i> <sub>488</sub> (a.u.) <sup>c</sup>	I488 increasing ratio (times, ×)	Entry	Mode <sup>a</sup>	Sample <sup>b</sup>	<i>I</i> <sub>405</sub> (a.u.) <sup>c</sup>	<i>I</i> <sub>488</sub> (a.u.) <sup>c</sup>	I488 increasin g ratio (times, ×)
1	Pure linker	1	$NA^d$	1.17		21 <sup>e</sup>	Pure linker	1	$NA^d$	1.17	
2	4-comp monomer solid	1.6	$\mathbf{NA}^d$	4.16	×3.6 from <b>1</b>	22	4-comp monomer solid	1.7	$\mathbf{NA}^d$	1.71	×1.5 from <b>1</b>
3	3-comp polymer sheet	P(1.6)	$NA^d$	22.3	×5.4 from <b>1.6</b>	23	3-comp polymer sheet	P(1.7)	$\mathbf{N}\mathbf{A}^{d}$	17.5	×10 from <b>1·7</b>
4	4-comp polymer sheet	P(1.6)	NA <sup>d</sup>	129	×31 from <b>1·6</b>	24	4-comp polymer sheet	P(1.7)	$\mathbf{N}\mathbf{A}^d$	40.5	×24 from <b>1·7</b>
5	Pure linker	2	79.3	7.10		25 <sup>e</sup>	Pure linker	2	79.3	7.10	
6	4-comp monomer solid	2.6	214	19.8	×2.8 from <b>2</b>	26	4-comp monomer solid	2.7	183	10.0	×1.4 from <b>2</b>
7	3-comp polymer sheet	P(2·6)	NA <sup>d</sup>	82.7	×4.2 from <b>2·6</b>	27	3-comp polymer sheet	P(2·7)	$NA^d$	45.1	×4.5 from <b>2·7</b>
8	4-comp polymer sheet	P(2·6)	$\mathrm{NA}^d$	87.3	×4.4 from <b>2·6</b>	28	4-comp polymer sheet	P(2·7)	$NA^d$	200	×20 from <b>2·7</b>
9	Pure linker	3	223	6.14		29 <sup>e</sup>	Pure linker	3	223	6.14	
10	4-comp monomer solid	3.6	244	9.44	×1.5 from <b>3</b>	30	4-comp monomer solid	3.7	$\mathbf{NA}^d$	14.5	×2.4 from <b>3</b>
11	3-comp polymer sheet	P(3·6)	$\mathbf{N}\mathbf{A}^{d}$	212	×22 from <b>3.6</b>	31	3-comp polymer sheet	P(3·7)	$\mathbf{N}\mathbf{A}^{d}$	120	×8.3 from <b>3·7</b>
12	4-comp polymer sheet	P(3·6)	NA <sup>d</sup>	221	×23 from <b>3·6</b>	32	4-comp polymer sheet	P(3·7)	$\mathbf{N}\mathbf{A}^d$	130	×8.9 from <b>3·7</b>
13	Pure linker	4	41.4	0.40		33 <sup>e</sup>	Pure linker	4	41.4	0.40	
14	4-comp monomer solid	4.6	252	16.3	×41 from <b>4</b>	34	4-comp monomer solid	4.7	$NA^d$	8.61	×22 from <b>4</b>
15	3-comp polymer sheet	P(4·6)	NA <sup>d</sup>	56.7	×3.5 from <b>4.6</b>	35	3-comp polymer sheet	P(4·7)	$\mathbf{N}\mathbf{A}^d$	57.7	×6.7 from <b>4·7</b>
16	4-comp polymer sheet	P(4·6)	$\mathrm{NA}^d$	61.3	×3.8 from <b>4·6</b>	36	4-comp polymer sheet	P(4·7)	$\mathbf{N}\mathbf{A}^d$	184	×21 from <b>4·7</b>
17	Pure L	5	1.57	0.059		37 <sup>e</sup>	Pure L	5	1.57	0.059	
18	4-comp monomer solid	5.6	160	8.99	×150 from <b>5</b>	38	4-comp monomer solid	5.7	24.9	0.310	×5.3 from <b>5</b>
19	3-comp polymer sheet	P(5·6)	NA <sup>d</sup>	12.3	×1.4 from <b>5·6</b>	39	3-comp polymer sheet	P(5·7)	$\mathbf{N}\mathbf{A}^{d}$	44.0	×140 from <b>5·7</b>
20	4-comp polymer sheet	P(5·6)	NA <sup>d</sup>	16.3	×1.8 from <b>5·6</b>	40	4-comp polymer sheet	P(5·7)	$\mathbf{N}\mathbf{A}^{d}$	52.5	×170 from <b>5·7</b>

<sup>*a*</sup> 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). <sup>*b*</sup> P denotes polymer. <sup>*c*</sup> *I*<sub>405</sub> and *I*<sub>488</sub> values were determined from CM emission intensities at 498 nm and 564 nm, respectively, at a constant area (10  $\mu$ m × 10  $\mu$ m) for all entries. <sup>*d*</sup> Not analyzable (> 255 a.u.) due to the detection limit of instrument ( $\lambda_{ex}$  = 405 nm). <sup>*e*</sup> Entry 21 = entry 1, entry 25 = entry 5, entry 29 = entry 9, entry 33 = entry 13, and entry 37 = entry 17.

Entry	Sample	I <sub>405</sub> (a.u.) <sup>a</sup>	I <sub>488</sub> (a.u.) <sup>a</sup>	<i>I</i> <sub>405</sub> increasing ratio (times, ×)	I <sub>488</sub> increasing ratio (times, ×)
1	Pure linker 5	358	0.152		
2	Linker <b>5</b> embedded in P4VP by casting	1720	86.6	×5 from <b>5</b>	×570 from <b>5</b>
3	Linker <b>5</b> embedded in PMMA by casting	415	18.3	×1.2 from <b>5</b>	×120 from <b>5</b>
4	Linker <b>5</b> embedded in P4VP by SPP (3-componet polymer sheet <b>P(5·6)</b> )	3220	90.9	×9 from <b>5</b>	×600 from <b>5</b>

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

 $^{a}$  I<sub>405</sub> and I<sub>488</sub> values were determined from PL spectra area integrated at 503–635 nm and 420–585 nm, respectively.



Fig. S9. 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 (1.6) (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)  $\lambda_{ex} = 405$  nm and (B)  $\lambda_{ex} = 488$  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)  $\lambda_{ex} = 405$  nm and (B)  $\lambda_{ex} = 488$  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)  $\lambda_{ex} = 405$  nm and (B)  $\lambda_{ex} = 488$  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)  $\lambda_{ex} = 405$  nm and (B)  $\lambda_{ex} = 488$  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  $\lambda_{ex} = 405$  nm and  $\lambda_{ex} = 488$  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(2.6), 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(4.7), and P(5.7) (third row, images B31–B40).



Fig. S19. Summary of Table S3. (A and B)  $I_{488}$  (green) and  $I_{405}$  (blue) values and emission enhancement (×, red) of pure linkers (1–5) (first row), 4-component monomer cocrystal solids (second row), and 3-component non-covalently crosslinked polymers (left) and 4component 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.<sup>2</sup> 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  $2 \cdot 6$  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  $5 \cdot 6$  at the linker/monomer ratios of (B) 1/1, (C)  $\frac{1}{2}$ , and (D)  $\frac{1}{4}$  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-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 cocrystal (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)  $(T_{d(10\%)} = 163 \text{ °C and } T_{d(50\%)} = 187 \text{ °C}).$ 

## 11. Emission of P4VP synthesized via solution phase radical polymerization



#### Solution-phase free 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  $\lambda_{ex} = 488$  nm (left) and  $\lambda_{ex} = 405$  nm (right).

# 12. Cartesian Coordinates

Atom Coordinates (Angstroms) X Y Z

## XB linker 1 (DBSb)

\_\_\_\_\_

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

#### XB linker 2 (DBTPA)

С	-1.160975	0.712222	-0.041328
С	-1.101314	-0.609582	0.051723
С	0.126014	-1.220204	0.022021
С	1.307374	-0.594911	0.007259
С	1.191068	0.765773	-0.056224
С	-0.005471	1.432212	-0.069796
Br	2.547601	1.924542	0.036426
С	2.463665	-1.353752	0.025050
С	-2.388710	1.330052	-0.095704
Br	-2.625700	-1.834213	0.042164
0	-2.518099	2.563956	-0.111145
0	3.560051	-0.914703	-0.104386
Н	0.145589	-2.371257	-0.053747
Н	0.019638	2.551562	-0.087185
Н	2.378193	-2.454633	0.071486
Н	-3.383533	0.726844	-0.185936

## XB linker 3 (BCA)

С	-4.383913 1.889593 -0.587498
С	-4.004489 0.736218 -0.005746
С	-4.882298 -0.229304 0.346719
С	-6.169925 -0.040865 0.000333
С	-6.647801 1.122383 -0.427424
С	-5.677516 2.021980 -0.866289
Br	-3.210081 3.367142 -0.876992
С	-6.984171 -1.076878 0.300351
С	-8.288729 -1.183613 0.203631
С	-8.936021 -2.298295 0.669835
0	-10.123818 -2.554171 0.644023
Н	-2.952193 0.595461 0.262512
Н	-4.534319 -1.125079 0.939066
Н	-7.675484 1.416758 -0.472700
Н	-5.970913 2.977708 -1.234431
Н	-6.495483 -1.853732 0.817369
Н	-8.911959 -0.401083 -0.195418
Н	-8.197415 -3.042343 1.099776

#### XB linker 4 (BDMB)

0	0.699114	-1.906154	0.099625
С	0.628303	-0.471118	0.142164
С	1.786542	0.226671	0.314789
С	1.874369	1.544682	0.239509
С	0.755199	2.203403	0.028503
С	-0.452445	1.620411	-0.108723
С	-0.534596	0.237946	0.045373
Br	0.824559	4.025759	-0.108421
С	2.978404	-0.382341	0.507374
0	-1.782581	-0.387896	-0.179776
0	4.104766	0.099822	0.635578
С	-0.357220	-2.711255	-0.437955
С	-2.885525	0.358970	-0.617721
Н	2.753053	2.108813	0.409169
Н	-1.358059	2.206937	-0.109019
Н	2.970896	-1.430521	0.515394
Н	-1.215505	-2.724889	0.272781
Н	-0.456471	-2.400025	-1.512353
Н	-0.022905	-3.829805	-0.461440
Н	-3.294678	1.132626	0.083890
Н	-2.636449	0.877268	-1.555822
Н	-3.711406	-0.397227	-0.704168

#### XB linker 5 (4BB)

С	1.080780 0.692801	0.132796
С	1.199529 -0.656870	0.206968
С	0.099212 -1.391775	0.007259
С	-1.091756 -0.737341	0.009447
С	-1.226708 0.577753	0.115441
С	-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
Н	0.082621 -2.467331	-0.122824
Н	-0.173848 2.389135	0.210763

## Monomer solid 1 6 (DBSb 4VP)

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

Н	-4.046874	-1.080690	-1.336564
н	0.807933	-2.248223	-2.476126
н	-0.084032	-0.471559	-0.082297
н	1.465012	0.758834	1.077864
Н	3.625949	1.449836	1.379539
Н	4.987632	-0.824501	-1.944771
Н	2.776693	-1.514334	-2.299893
Н	-9.215825	1.454170	-0.872715
Н	-6.743233	0.424777	-1.400404
Н	-8.128565	-3.316709	-1.542899
н -	10.483695	-2.613363	-0.957703
н -	-11.147422	1.064859	-0.154151
н -	-13.120491	-0.101529	0.110065
н -	-12.372697	-1.739401	-0.432651
Н	6.966102	2.658263	4.066787
Н	6.379049	2.017826	2.197233
Н	9.805063	1.626782	0.574638
Н	10.771709	2.494034	2.418965
Н	8.797105	3.228462	5.440546
Н	11.016631	3.563255	6.063861
Н	11.607702	3.077090	4.354072
Monon	ner solid 1	7 (DBSb N	VP)
C	2 217209	2 109577	0.022245
č	-3.31/308	-3.1903//	-0.023343
c	-2.439048	-3.434913	-1.002930
c	-1.380/0/	-2.041380	-1.183841
č	-1.1/2/39	-1.33080/	-0.410003
c	2 120048	-1.324403	0.300338
c	0.000203	0.785112	0.658585
c	0.207381	0.320046	0.007623
c	1 278116	1 102537	0.257685
c	1.501688	2 187844	0.516730
c	2 640586	2.187844	0.329563
c	3 51 5790	2 751361	-0.653621
c	3 330351	1 679956	-1 437776
c	2 275782	0.872434	-1 237455
Br	4 998688	3 894230	-0.929093
Br	-4 807800	-4 333069	0.246739
N	-8.037600	-4 385923	-0.329686
C	-7 245024	-4 688160	0.615978
Ĉ	-7 659128	-4 115201	1 965441
č	-9.138184	-3.819005	1.725974
Ĉ	-9.159945	-3.571808	0.210851
Ō	-6.238977	-5.383240	0.496352
С	-8.008479	-4.658599	-1.571724
С	-8.869030	-4.284768	-2.530483
Ν	7.729753	4.840482	0.611019
С	7.381437	4.522754	-0.568640
С	8.307399	3.507088	-1.225602
С	9.567666	3.654695	-0.375559
С	8.980596	4.116511	0.965817
0	6.407045	4.978466	-1.162236
С	7.202624	5.625700	1.461528
С	7.608534	5.900213	2.710281
Н	-2.569720	-4.328148	-1.664309
Н	-0.695407	-2.899702	-2.007537
H	-1.989235	-0.466865	1.251316
н	-3.842050	-1.897/407	1.573904
H	0.542/53	-1.116832	-1.496838
H	-0.335320	0.660422	0.831018
H	0.902219	2.444265	1.340480
H	2.//04/8	3.8/8858	0.989932
п	4.038/21	1.431402	-2.232391
п u	2.192130	4 921426	2 800226
п u	7 001527	2 172711	2.800220
н	-9 525070	-2 961826	2 321012
H	-9 739491	-4 727580	1 972705
н	-10 158264	_3 873871	-0 182464
Ĥ	-8 978474	-2 493254	-0.012701
Ĥ	-7.150974	-5.278060	-1.885669
H	-8,705173	-4,600542	-3.573144
H	-9,752230	-3,656486	-2.352573
Н	7.869869	2.487748	-1.112539
н	8.481059	3.726639	-2.302903
н	10.209981	4,459875	-0.808123
н	10.168842	2.720966	-0.298634
Н	8.732540	3.237930	1.608253
Н	9.734643	4.756525	1.480019
Н	6.287005	6.132980	1.112312
Н	7.037625	6.606868	3.333476
Н	8.493162	5.451016	3.181530

Mo	nomer solid 2	6 (DBTP.	A 4VP)
C	1 027520	1 0207/	15 5 000605
c	-1.937320	-1.92072 -1.02904	-5.908685 2 -5.090553
Ν	-3.042504	-1.25510	-3.958658
С	-3.144282	-2.49466	-3.657522
C	-2.5888/3	5 -3.49110 3 18072	08 -4.376830 09 -5 477641
c	-1.439655	-4.19098	-6.221913
С	-0.759962	-4.21353	33 -7.398647
C	-0.537734	-0.16042	24 -1.349787
c	1.351892	-0.19733	5 0.031129
Ċ	0.822779	0.77502	8 0.783508
С	-0.321689	1.36077	6 0.451322
С	-1.001381	0.86790	6 -0.571805
Br	1.791151	1.38586	9 2.341928
С	1.344591	-1.58845	3 -1.795707
Br	-1.812350	-0.68437	2 -2.686924
С	1.493027	2.56383	5 5.525134
N	2.039199	1.87863	5 3.774781
С	2.987961	3.13361	5 3.575191
С	2.385799	4.18638	0 4.223278
С	1.641196	3.86821	6 5.267612 7 6.129644
c	1.334766	6.02034	2 6.190383
0	-2.028285	5 2.90776	0.914252
0	2.524632	-1.87788	-1.701152
H U	-1.666391	-1.64756	6 -6.935979 6 5.380577
Н	-3.700888	3 -2.79053	6 -2.745298
Н	-2.770496	-4.53759	-4.032212
Н	-1.580686	5 -5.21760	4 -5.952720
Н	-0.470985	5 -5.14084	8 -7.897103
Н	2.361471	-0.68016	5 0.400037
Н	-2.079642	1.10705	9 -0.641999
Н	-0.333974	2.89382	5 1.977521
H U	0.717925	-1.96418	9 -2.616200 5 6.407530
п Н	1.990081	0.50991	5 6.407550 9 5.069575
Н	3.670853	3.44630	7 2.835681
Н	2.682721	5.17092	3 3.949280
Н	0.550963	4.32250	9 6.999186 5 7.006452
п Н	1 842659	6 52190	0 5 375104
Mo	nomer solid 2	7 (DBTP.	A NVP)
С	-5.925369	1.876506	-0.669067
c	-0.043733	0.039034	-0.133376
č	-8.325749	0.004464	-1.287650
С	-7.926166	1.239565	-1.647470
С	-6.948320	2.143172	-1.465662
Br	-8.636542	-1.814875	-0.589635
С	-5.059825	0.228357	0.722316
Br	-4.552257	3.171373	-0.427275
0	-8.968795	2.753165	-3.085072
N	-1.336930	3.201899	-0.395875
С	-2.234908	4.006166	-0.797338
С	-1.988333	4.551734	-2.197284
С	-0.497664	4.270561	-2.374034
0	-3.223202	4.342382	-0.149774
С	-1.206026	2.557498	0.693087
С	-0.240936	1.695145	1.045589
N C	-6.875050	-3.825677	1.166594
č	-8.766269	-3.358775	2.466635
С	-7.748097	4.020052	3.392712
C	-6.449390 .	3.847314	2.592558
U C	-8.776160	-3.47/6166	0.072355
č	-4.694684	4.273442	0.200394
Н	-6.809337	-0.928604	0.164863
Н	-6.939885	3.131048	-1.954455
Н Н	-9.751271 -4.210224	0.982903	-2.702268
Н	-2.594401	3.963811	-2.925541
Н	-2.240480	5.632594	-2.281243
H	0.088126	5.139420	-1.986884
н	-0.199346	4.080666	-3.429546

H H H H H H H H H H H H H H H H	-0.476308         2.107226         -2.016900           0.741638         3.074068         -1.064283           2.005847         2.737020         1.431759           -0.269898         1.208509         2.033549           0.601662         1.417265         0.398183           -8.837195         -2.264179         2.667587           -9.776625         -3.821452         2.529452           -7.992943         -5.105414         3.492824           -7.706584         -3.567858         4.409044           -5.957237         -2.880707         2.853801           -5.767823         -4.693556         2.841225           -6.407656         -4.024456         -0.767991           -4.069058         -4.438772         -0.495728           -4.171034         -4.299067         1.360887
Mor	nomer solid <b>3 6</b> (BCA 4VP)
ССNССССССССССВСССОНННННННННННН	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$
Mor	nomer solid <b>3 7</b> (BCA NVP)
СССССС ВСССОИСССООССННННННННННННН	$\begin{array}{llllllllllllllllllllllllllllllllllll$

Н	-2.868301 -1.212322 -2	.158839
Н	-4.824122 0.117432 -2	.517223
Η	-5.384712 -0.074636 -0	.749064
Mo	nomer solid <b>4</b> 6 (BDMB	1VP)
WIO		••••)
С	-5.451254 -3.500149	2.093772
C	-6.653439 -3.795929	1.618172
N	-6.950738 -3.787644	0.387069
c	-0.02040/ -3.8/84/9	-0.491555
Ċ	4.733831 -3.020492	1 162063
Č	-3 156061 -3 116728	1.102003
Č	-2 782881 -2 773977	2 773835
č	-7 684043 -0 210235	-0.001820
č	-6.874304 0.628202	0.686534
С	-7.038167 2.010303	0.653207
С	-7.982303 2.503998	-0.162739
С	-8.876964 1.732823	-0.805474
С	-8.719268 0.381851	-0.678551
Br	-7.461142 -2.065029	0.073572
С	-6.181472 2.642191	1.442003
0	-6.076318 3.851044	1.598598
0	-8.118304 3.868935	-0.251688
С	-7.187482 4.524269	-1.103/43
0	-9.96/239 2.236490	-1.55/146
с и	-11.29443/ 1.03219/	-1.309121
н	-7.465810 -4.114061	2 284931
н	-6 311163 -4 202405	-1 497820
н	-3.882860 -3.743013	-0.893953
Н	-2.417606 -3.075345	0.737946
Н	-1.682097 -2.566745	3.004231
Н	-3.419160 -2.683502	3.694244
Н	-5.993044 0.210152	1.134611
Н	-9.458840 -0.202243	-1.254473
Н	-5.440024 2.002760	1.971147
Н	-7.419958 4.415346	-2.187546
Н	-7.172575 5.577545	-0.854129
Н	-6.172177 4.044452	-0.992549
H	-11.919/02 2.43/201	-1./51965
п	-11.55/840 0./21/29	-1.85/490
п	-11.349070 1.412638	-0.204090
Mo	nomer solid 4 7 (BDMB	NVP)
C	5 211007 0 022614 0	127522
Č	-5.082972 -1.261383 0	317647
č	-6 109351 -2 049853 0	688843
č	-7.393821 -1.606433 0	.619781
С	-7.628057 -0.343820 0	161212
С	-6.572839 0.416544 -0	197249
Br	-3.867880 1.089135 -0	.649150
0	-8.378444 -2.490478 1	.011268
0	-8.913721 0.139152 0	082144
C	-5.782517 -3.300838 1	.133/5/
N	-0.49/409 -4.190328 1	.328380
C	-0.092808 $1.323242$ $-01.447357$ $1.460150$ $1$	000577
Č	-0.916037 0.769008 -2	347502
č	-0.002080 -0.287141 -1	.729487
Č	0.424343 0.401933 -0.	425101
С	-0.747589 1.830455 1.	079193
С	0.102636 1.659500 2.	102553
С	-9.162370 1.461145 -0	.335559
С	-9.754624 -2.224934 0	.898235
0	-2.482472 2.120440 -1	.129077
Н	-4.036439 -1.607943 0	.369604
H	-6.716275 1.442604 -0	.568013
H	-4.68/502 -3.525847 1	.132361
H U	-1./21120 0.331294 -2	.7/8930 040421
н и	-0.333368 1.312081 -2	380516
п Ц	-0.602473 -1.200878 1	499460
н	0.598859 _0.378607 0	351785
H	1.359675 0.990043 -0	.585073
Н	-1.607944 2.499900 1	249847
Н	-0.076546 2.172017 3	061115
Н	1.001967 1.030558 2.	054144
Η	-10.263144 1.623364 -	0.298225
Н	-8.686816 2.186522 0	361676
Н	-8.833411 1.606373 -1	.388654
H	-10.295063 -3.137907	1.236123
Н	-10.056425 -1.400938	1.581004

Н -10.037294 -2.051334 -0.163302

Monomer solid 5 6 (4BB 4VP) (Linker / monomer ratio = 1/1)

С	-4.917795 3.191257 -0.556843
С	-5.973478 4.025285 -0.609949
С	-7.223649 3.532382 -0.626633
С	-7.523366 2.222608 -0.504430
С	-6.506309 1.358998 -0.390762
С	-5.237802 1.875031 -0.429184
Br	-6.794156 -0.529870 -0.090219
Br	-9.401396 1.669843 -0.454754
Br	-5.822007 5.903184 -0.761171
Br	-3.040596 3.770234 -0.542243
С	-9.628199 -2.200274 0.040876
С	-8.450597 -2.309277 -0.607538
Ν	-7.329403 -2.304998 0.001412
С	-7.399036 -2.501495 1.272480
С	-8.507796 -2.365036 2.041005
С	-9.686640 -2.225180 1.429365
С	-10.824000 -2.204010 2.113610
С	-12.128875 -2.097505 1.909939
Н	-8.104551 4.220120 -0.571158
Н	-4.381824 1.211427 -0.287007
Н	-10.625823 -2.194921 -0.506909
Н	-8.467405 -2.524833 -1.762636
Н	-6.427058 -2.767196 1.806665
Н	-8.403870 -2.540157 3.149769
Н	-10.704431 -2.401293 3.203802
Н	-12.811024 -2.072569 2.829985
Н	-12.479091 -1.789395 0.868261

Monomer solid 5 6 (4BB 4VP) (Linker / monomer ratio = 1/2)

С	-5.943212 1.284198 0.766550
С	-5.665633 0.196883 1.547591
С	-5.219331 -0.887683 0.929190
С	-4.866861 -0.900875 -0.352566
С	-5.103111 0.251811 -1.071139
С	-5.673047 1.340065 -0.543155
Br	-5.091326 -2.383398 2.086073
Br	-6.071100 2.856483 -1.637767
Br	-4.272866 -2.421396 -1.332622
Br	-6.728760 2.736262 1.673594
N	-5.001417 -4.007227 2.926654
С	-3.879641 -4.460737 2.491623
С	-3.669680 -5.332451 1.548055
С	-4.728951 -5.963475 1.041744
С	-5.915623 -5.698638 1.629065
С	-6.014216 -4.759747 2.558637
С	-9.104770 4.896071 -2.195088
С	-8.069669 5.387216 -1.483182
С	-6.831948 5.103599 -1.751005
Ν	-6.464710 4.305573 -2.656820
С	-7.412876 3.942129 -3.438128
С	-8.754350 4.055750 -3.212690
С	-4.690054 -6.886830 0.013786
С	-10.411722 5.287232 -2.122219
С	-10.931838 5.779919 -0.988136
С	-3.531158 -7.267430 -0.580344
Н	-5.843253 0.028303 2.660148
Н	-4.894816 0.189745 -2.160486
Н	-2.894864 -4.055453 2.893094
Н	-2.657987 -5.537335 1.236618
Н	-6.831497 -6.166843 1.237563
Н	-6.932732 -4.715525 3.138862
Н	-8.223942 6.235262 -0.712221
Н	-6.018153 5.806815 -1.323925
Н	-7.063390 3.440599 -4.311604
Н	-9.522776 3.732608 -3.969862
Н	-5.650712 -7.424168 -0.217317
Н	-11.153809 4.976024 -2.842768
Н	-12.024071 5.751168 -0.806062
Н	-10.379046 5.888433 -0.081961
Н	-3.524357 -8.105325 -1.275401
Н	-2.592153 -6.704342 -0.442668

C	-0 822879	-2 496312	5 299171
č	0.022079	2.150512	1.2////
C	0.304674	-2.16058/	4./41233
Ν	0.695941	-2.669004	3.610125
C	0.002001	2 600064	2.050021
C	-0.002001	-3.009004	5.058851
С	-1.231794	-3.876821	3.527110
C	-1 715358	-3 346151	4 672939
0	-1.715556	-5.540151	4.072757
С	-2.996227	-3.646440	5.154618
C	2 451482	3 028767	6 260600
č	-3.431462	-3.028707	0.200090
C	-0.527826	-0.065609	1.142278
C	-1.012353	1 166323	1 402487
č	1.502222	1.052/20	0.450705
C	-1.582322	1.853674	0.450/95
С	-1.671115	1.431033	-0.803036
c.	1 220022	0.221674	1 172200
C	-1.220025	0.2210/4	-1.1/2290
С	-0.634239	-0.542503	-0.163410
D.	1 126122	0 617122	2 865421
DI	-1.130123	-0.01/155	-2.805451
Br	-2.567330	2.556130	-1.953331
Br	-1 278317	1 902687	3 187044
DI	1.270517	1.902007	5.107011
Br	0.2217/2	-1.295023	2.499584
C	-0 621086	-0 366688	-6 257099
č	1 45 4707	0.072572	5.224026
C	-1.454/9/	-0.8/33/3	-3.334830
Ν	-1.053862	-1.629359	-4.420680
C	0 111227	2.074492	4 500440
C	0.11133/	-2.0/4482	-4.322449
С	1.049733	-1.644972	-5.393471
C	0.682434	0.675466	6 242202
C	0.002434	-0.075400	-0.243372
С	1.637912	-0.233844	-7.053312
C	1 472334	0.626244	-8 044095
č	1.172331	0.020211	6.0011095
C	-1.494842	0.781515	6.339517
C	-2.048805	1 564772	5 455042
Ň	1 4777777	2.500024	4.962624
IN	-1.4/////	2.580834	4.862634
С	-0.416686	2.907715	5.525170
c.	0.210490	2 266662	6 409071
C	0.219480	2.200003	0.4980/1
С	-0.296802	1.081168	6.873520
C	0.210166	0 201227	7 047608
C	0.210100	0.391237	/.94/008
С	1.251850	0.742524	8.736187
C	-1 877811	4 680083	-4 392276
~	-1.077011	4.000000	-4.372270
C	-2.605214	4.664420	-3.21/8/0
N	-3470092	3 780364	-2 939735
~	2.750276	2.076476	2.005400
C	-3./582/6	3.0/64/6	-3.985422
С	-3.093580	2.963380	-5.149484
C	2 087725	2 772202	5 296910
C	-2.08//25	5.775505	-3.380819
С	-1.382182	3.849868	-6.528931
C	1 590192	2 052246	7 602946
C	-1.369165	5.055240	-7.003840
н	-1.028625	-2.154464	6.265477
н	1.065065	-1 511118	5 188513
11	1.005005	1.015041	2.101241
н	0.4/2993	-4.215841	2.191341
Н	-1.927290	-4.558114	3.010103
11	2.520544	4 45 40 41	4 (2)((15
н	-3.338344	-4.454241	4.626615
Н	-4.414923	-3.454133	6.614832
ы	2 042250	2 227507	6 000185
п	-2.942230	-2.52/59/	0.909185
Н	-1.828056	2.897851	0.702590
н	-0 312469	-1 576507	-0.390162
11	0.001000	0.072455	3.375102
н	-0.991908	0.2/3455	-/.0/5490
Н	-2.533077	-0.679978	-5.404512
ц	0.308101	2 081202	3 860032
11	1.00225	2.701302	5.007752
н	1.983251	-2.178777	-5.448337
н	2 649758	-0.731172	-7 130260
11	2.049750	-0.751172	-7.130200
Н	2.359864	0.813911	-8.739351
Н	0 546984	1 245517	-8 142148
11	2,000,700	0.0(7072	6 702177
п	-2.088/88	-0.00/2/3	0./921//
Н	-3.100156	1.467752	5.167074
н	-0 127510	3 080205	5 302585
11	-0.12/310	3.709293	5.502565
Н	1.121976	2.838339	6.933716
н	-0.360439	-0 508680	8 268402
11	1.500438	0.000000	0.200402
Н	1.588014	0.196971	9.606025
Н	1.766828	1.686880	8.484136
	1.004020	E 470510	4 470720
н	-1.094828	5.4/8518	-4.4/9/38
Н	-2.404528	5.449266	-2.464200
ц	4 700709	2 404407	2 826110
n	-4./00/08	2.49449/	-3.620110
Н	-3.498418	2.261917	-5.860951
н	-0.628289	4 630548	-6 510160
11	0.020209	1.050540	5.510100
н	-2.352768	2.347124	-/.508090
Н	-0.990361	3.031813	-8.545197

Monomer solid 5 7 (4BB NVP) (Linker / monomer ratio = 1 / 4)

С	0.811255	-0.092620	0.467609
С	0.815198	-1.279413	-0.169445
С	-0.349754	-1.842081	-0.534135
С	-1.519404	-1.233181	-0.271969
С	-1.523516	-0.047509	0.366876
С	-0.358149	0.515523	0.730673
Br	-3.125224	0.898745	0.782679
Br	-3.116738	-2.110274	-0.831981
Br	2.428488	-2.216002	-0.579904
Br	2.414453	0.787836	1.015316
Ν	5.131640	3.283552	0.777384
С	4.353581	2.303621	0.538599
С	4.050468	2.187613	-0.960571

Monomer solid 5 6 (4BB 4VP) (Linker / monomer ratio = 1 / 4)

С	5.207503 2.958348 -1.591179	С	9.447876 8.302368 -1.090732
С	5.510937 3.973359 -0.485701	С	8.848234 4.102581 -2.079246
0	3.977786 1.554848 1.448462	С	8.076841 3.028129 -2.340825
С	5.600437 3.728510 1.874311	С	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	9.9/4692 4.015992 -1.364380
C	5.504110 -1.662530 -2.113656	Br	8.306922 5.850327 -2.678897
C	6.83089/ -1.083/2/ -1.6280/5	Br	11.008511 5.546030 -0.984521
C	0.5181/8 -0.//2114 -0.158252	Br	/.388552 0.341428 -2.220691
C	4.000/14 -5.034063 -0.85/200	Br	10.319354 0.183533 -0.388646
c	5.209521 -1.914249 1.402034	C	0.380232 4.848313 2.072811
N	5.790296 -1.551090 2.522565	C	5.596610 4.564047 1.776770
C	5.090700 -4.597277 0.295841	N	5.794582 5.900457 0.705445 6.007721 2.251828 0.476851
Ċ	-6.267008 -2.370043 0.399854	C IN	7 797975 3 572228 1 351390
c	-7.034480 -3.366194 1.265947	C	7 637006 4 417136 2 392839
č	-5 977857 -4 456169 1 493659	Č	1 108494 8 776662 -2 189184
ŏ	-4 653624 -2 911247 -1 291103	Č	5 238737 4 951315 4 840185
č	-4.356600 -5.393813 0.018238	č	0.502253 7.374955 -1.978284
Ē	-4.219725 -6.548040 0.687935	Č	-0.297787 6.919051 -3.239373
N	-4.986012 3.169312 -0.586806	Č	0.075486 5.557658 -3.774124
C	-5.186133 2.079914 0.035297	Č	1.229606 5.233825 -4.347225
Ĉ	-6.171498 1.149782 -0.658911	Ċ	1.465852 3.971381 -4.784969
С	-6.876107 2.108012 -1.616435	Ν	0.590344 3.064345 -4.747467
С	-5.794992 3.175486 -1.835724	С	-0.553780 3.357829 -4.306997
0	-4.660194 1.768611 1.100964	С	-0.837147 4.565705 -3.742931
С	-4.249352 4.170514 -0.316865	С	2.401786 1.495566 -0.798211
С	-4.057728 5.287105 -1.035132	С	2.857502 0.716134 0.156216
Н	-0.344906 -2.814625 -1.055286	С	3.069730 -0.582295 -0.056822
Н	-0.360375 1.489350 1.249657	С	2.855764 -1.120471 -1.300903
Н	4.027829 1.139902 -1.337112	С	2.391846 -0.348426 -2.293494
н	3.087270 2.703750 -1.187277	С	2.095886 0.948866 -1.981293
Н	4.957899 3.426435 -2.569777	Br	2.017096 3.324827 -0.465354
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Н	6.592230 4.237835 -0.544955	Br	3.709438 -1.496073 1.592649
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Н	5.295888 3.166482 2.773688	С	4.548125 -7.442899 -0.134206
Н	6.718492 5.047229 3.101231	С	5.215592 -6.946880 -1.431155
Н	6.767448 5.446328 1.282040	С	6.443444 -6.041393 -1.218750
Н	5.632759 -2.453629 -2.886046	С	7.277400 -5.839211 -2.465608
Н	4.835827 -0.860720 -2.505016	С	8.396458 -4.792029 -2.289795
Н	7.169477 -0.194744 -2.206311	С	7.718452 -3.410987 -2.213534
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Н	7.453408 -0.899617 0.434938	С	10.511259 -3.993624 -1.067190
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H	6.576965 -0.568485 2.450329	С	3.602542 -6.268368 0.347137
н	-5./28531 -1.623431 1.029114	C	2.460/58 -8.7/6508 -0.966546
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H	-/.429981 -2.92/308 2.209394	C	3.69/366 -11.00/133 -0.391880
п	-5.570908 -4.254805 2.408010 6 500422 5 433048 1 616108	C	7 200502 2 820544 1 052120
и Ц	2 747418 5 272512 0 802704	C	6 570000 1 722102 1 162265
н	-3 527814 -7 321619 0 318480	N	6.243036 -1.087829 -2.232195
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Н	-6.870770 0.669095 0.061208	Č	12.960216 -4.987575 -2.586828
н	-7.758142 2.559825 -1.100863	С	13.617175 -3.853030 -2.744772
Н	-7.221537 1.626193 -2.558608	С	13.927599 -3.235891 -3.952267
Н	-5.144291 2.902710 -2.700822	Ν	13.575360 -3.865118 -5.030994
Н	-6.297402 4.149852 -2.037169	С	13.030620 -4.989753 -4.951326
Η	-3.695795 4.089545 0.634288	С	12.652559 -5.533645 -3.783068
Η	-3.377654 6.071067 -0.665584	С	2.705445 -6.517503 1.589932
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		C	3.507907 -7.100054 2.723131
Poly	mer P(5·6) (P(4BB·4VP)) (linker/monomer unit ratio = $1/2$ )	С	4.741507 -6.170310 3.019337
		C	4.669815 -4.678674 2.894749
		C	5.625537 -3.936628 2.326019
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č	5 620391 10 088714 0 329661	C	3.070700 -2.741307 3.089003 2.710242 4.000761 2.610455
č	6.918511 9.297121 -0.825001	C	5./17243 -4.070/01 5.010455 5.466106 2.421021 5.144069
č	7 880014 8 800526 0 935912		6 701350 3 271905 6 120400
č	9 167021 8 344218 0 230030		7 170092 1 814826 6 260000
č	7.289290 7.604630 1.709068	C	14 628380 -6 857764 -1 102114
č	6.893505 8.018132 3.138803	c c	15 648187 -7 676690 -0 380751
č	5.741152 7.134892 3.724494	c c	15.062055 -9.002050 0.293204
č	6.229100 5.677860 3.922626	c c	7 806023 1 265304 5 164170
č	4.077465 8.158761 -1.971491	c c	14 251597 -8 923784 1 547475
č	1.994114 9.274548 -1.001983	c c	9 104814 1 527544 4 947214
č	3.842234 6.841494 -1.588028	c c	9 759933 1 083222 3 813971
Ċ	4.364578 5.889710 -2.363723	N	9.160773 0.442137 2 910822
Ν	5.026575 6.022886 -3.418884	Ċ	7.877194 0.345851 3.027666
С	5.228245 7.179088 -3.807104	č	7.233284 0.546322 4.196666
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Ν	11.533283 7.326419 -0.657829	Ċ	13.944752 -8.674659 3.871969
С	10.697614 7.899681 -1.434792	С	14.678876 -8.544416 2.782070

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Ċ	11 145316 -5 688908 3 913896	н	7 741717 -6 828962 -2 810121
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č	9 551 554 -4 134582 3 362922	н	8 743418 -4 993771 -0 142554
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Br	9.6/1181 -1.263036 3.362984	H	10.1/9889 -3.024349 -0.797286
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Н	5.488960 11.033747 -0.252607	Н	1.976515 -7.864170 -1.233566
Н	5.824769 10.317942 1.431141	Н	0.808960 -10.107509 -1.578545
Н	6.570172 8.510459 -0.810752	Н	4.187845 -11.960683 -0.239838
Η	7.498804 10.076081 -0.697147	Η	5.363542 -9.914754 0.185460
Η	8.217087 9.555439 1.590699	Н	7.575171 -3.095101 0.022861
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ц	1 604662 10 248654 0 752668	ц	2 211522 5 540172 1 842222
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п	5.557080 0.512578 -0.044805 4.204002 4.706108 -2.078265	п	13.243933 -0.344632 0.033030
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н	4.998946 9.254525 -3.519558	н	3.81/020 -8.105885 2.519911
H	10.081/4/ 8.055993 2.135009	Н	5.031417 -6.431925 4.133020
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Η	4.396798 4.995767 1.884641	Η	4.550149 2.936809 5.537520
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Η	8.817301 3.054516 1.175797	Н	7.473149 3.977079 5.779734
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Η	5.271143 -7.651770 0.646155	Н	14.300833 -8.487568 4.859048
Η	4.458578 -6.348767 -2.054050	Н	15.686387 -8.314086 2.837337
Η	5.512229 -7.810842 -2.042125	Н	13.019664 -4.867761 4.358449
Н	7.011927 -6.495873 -0.360647	Н	8.468577 -3.895534 3.121643

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## **Author Information**

ORCID of Hong Tho Le: 0000-0002-0043-1404

ORCID of Atsushi Goto: 0000-0001-7643-3169