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The Effect of Polymer Molecular Weight on the Performance of PTB7-Th:O-IDTBR Non-Fullerene Organic Solar Cells

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Photovoltaic Performance

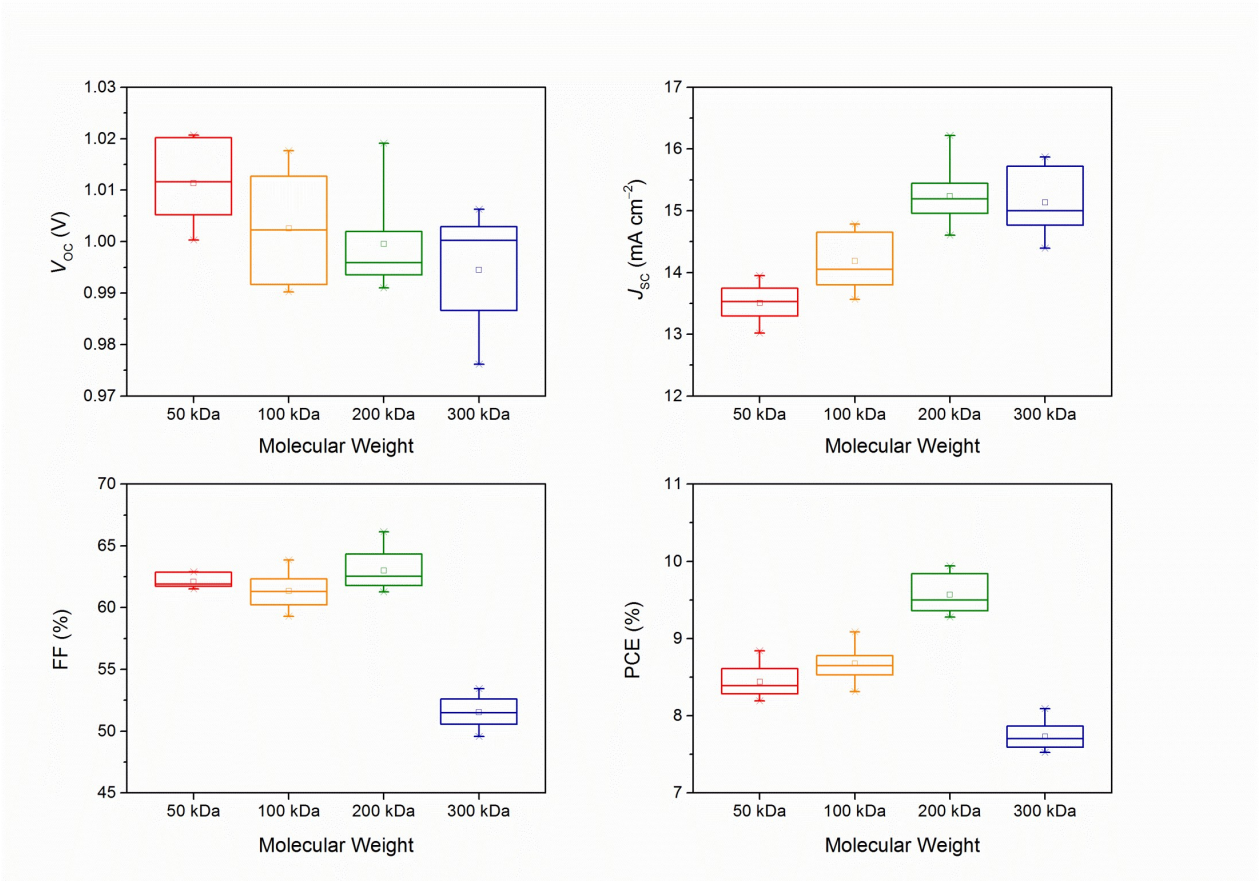

Figure S1. Performance analysis of PTB7-Th:O-IDTBR solar cells with a different molecular weight of PTB7-Th over ten photovoltaic devices presented as box plot diagram for the characteristic photovoltaic parameters (V_{OC}, J_{SC}, FF, PCE). The horizontal lines denote the 25th, 50th, and 75th percentiles. The whiskers are given by the 5th and 95th percentile values. The highest and the lowest values observed are denoted with a cross, while the mean average values are represented as an empty square.

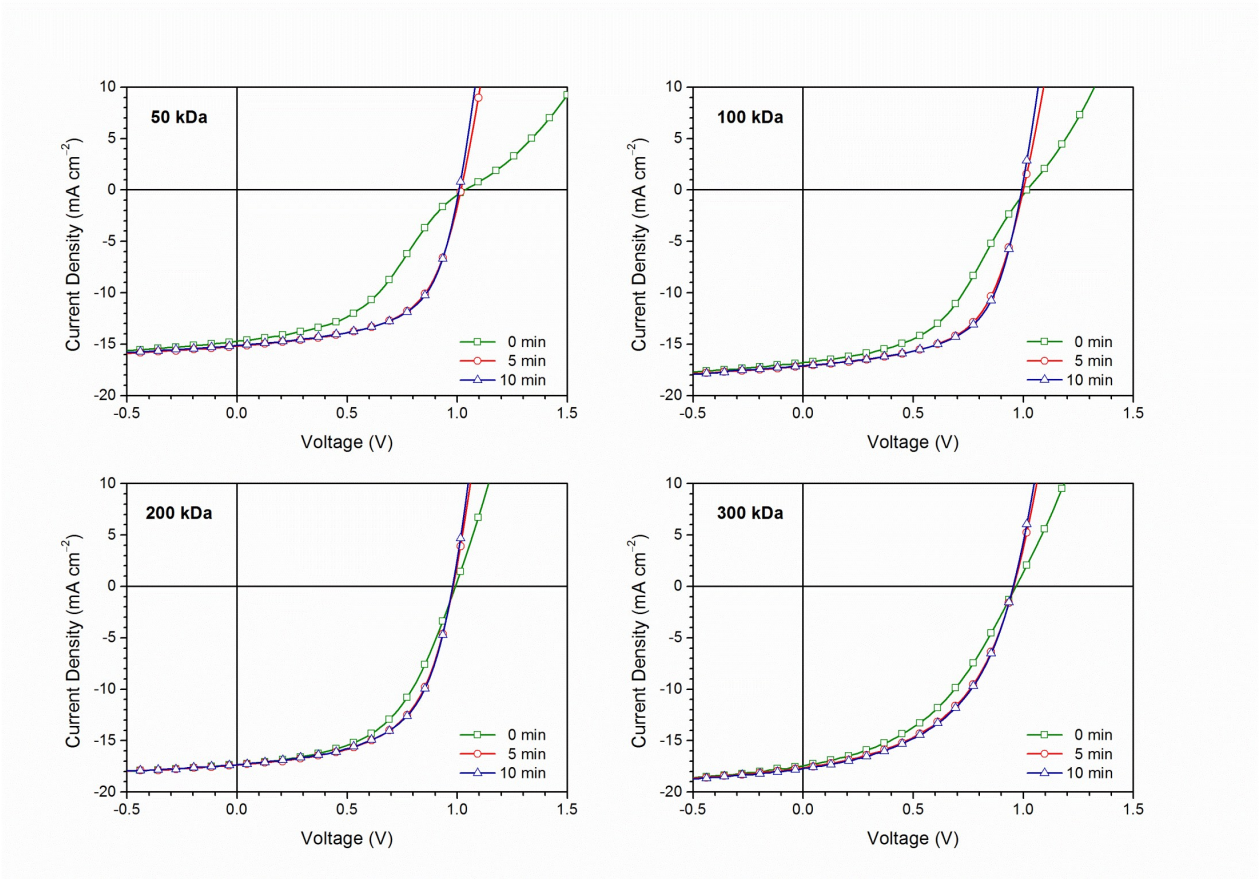

Figure S2. Current density−voltage (*J*−*V*) curves of PTB7-Th:O-IDTBR solar cells with a different molecular weight of PTB7-Th under illumination. The *J*−*V* curves were obtained after light soaking treatment for 0 min, 5 min and 10 min under continuous illumination with a Dedolight DLH400D xenon lamp (1000 W m^{-2}, AM 1.5 G).

UV-Vis Spectroscopy

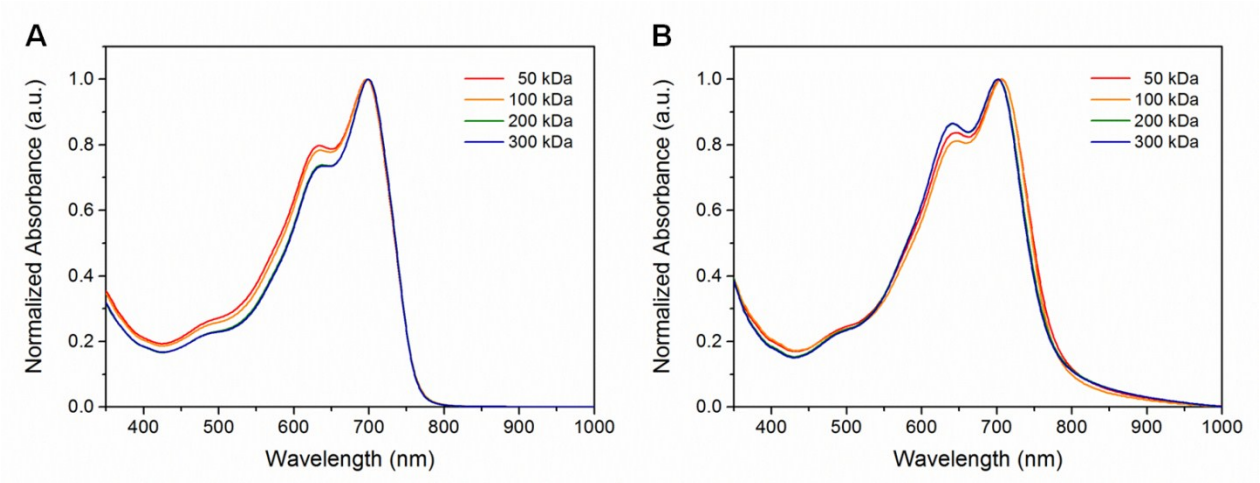

Figure S3. Normalized UV-Vis absorption spectra of (A) PTB7-Th solutions in chloroform and (B) PTB7-Th thin films deposited from *ortho*-dichlorobenzene with a different molecular weight.

Table S1. Optical properties of PTB7-Th with different molecular weight

Molecular Weight	$\lambda_{max,sol}$ **[nm]**	$\lambda_{max,film}$ **[nm]**	**α at** λ_{max} **[10^5 cm^{-1}]**	$\lambda_{onset,film}$ **[nm]**	$E_g^{opt\ a)}$ **[eV]**
50 kDa	697	706±0	1.77±0.02	781±2	1.59±0.00
100 kDa	697	706±1	1.86±0.16	781±2	1.59±0.00
200 kDa	699	703±2	1.56±0.11	781±4	1.59±0.01
300 kDa	699	703±1	1.54±0.10	781±3	1.59±0.01

a) The optical bandgap was determined from the onset of the thin film absorption spectra. Values for thin films were averaged over three samples.

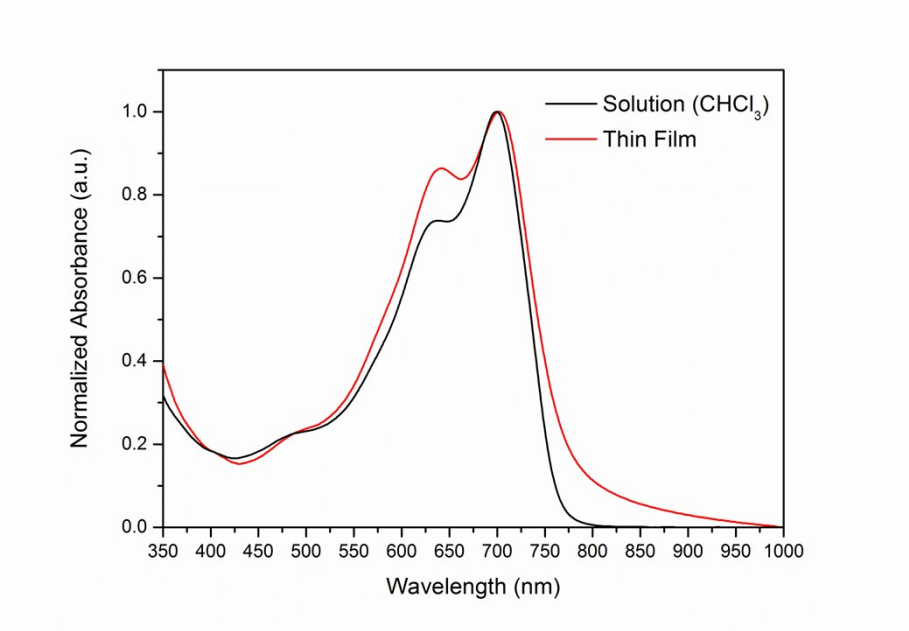

Figure S4. Normalized UV-Vis absorption spectra of a solution (in chloroform) and a thin film of PTB7-Th (200 kDa).

The difference in molecular weight has a negligible impact on the absorption properties of solution (in chloroform) and thin film samples (Figure S3). It can be therefore concluded that the effective conjugation length of PTB7-Th is already saturated, which is suggested to be below 50 kDa.[1,2] Comparing the absorption spectra of solution and thin film samples, a marginal bathochromic shift of the absorption maximum (4−9 nm) is observable, as reported previously (Figure S4).[3] This is considerably different to homopolymers like P3HT, where absorption spectra are typically red-shifted from solution to solid-state.[4]

Charge Carrier Mobility

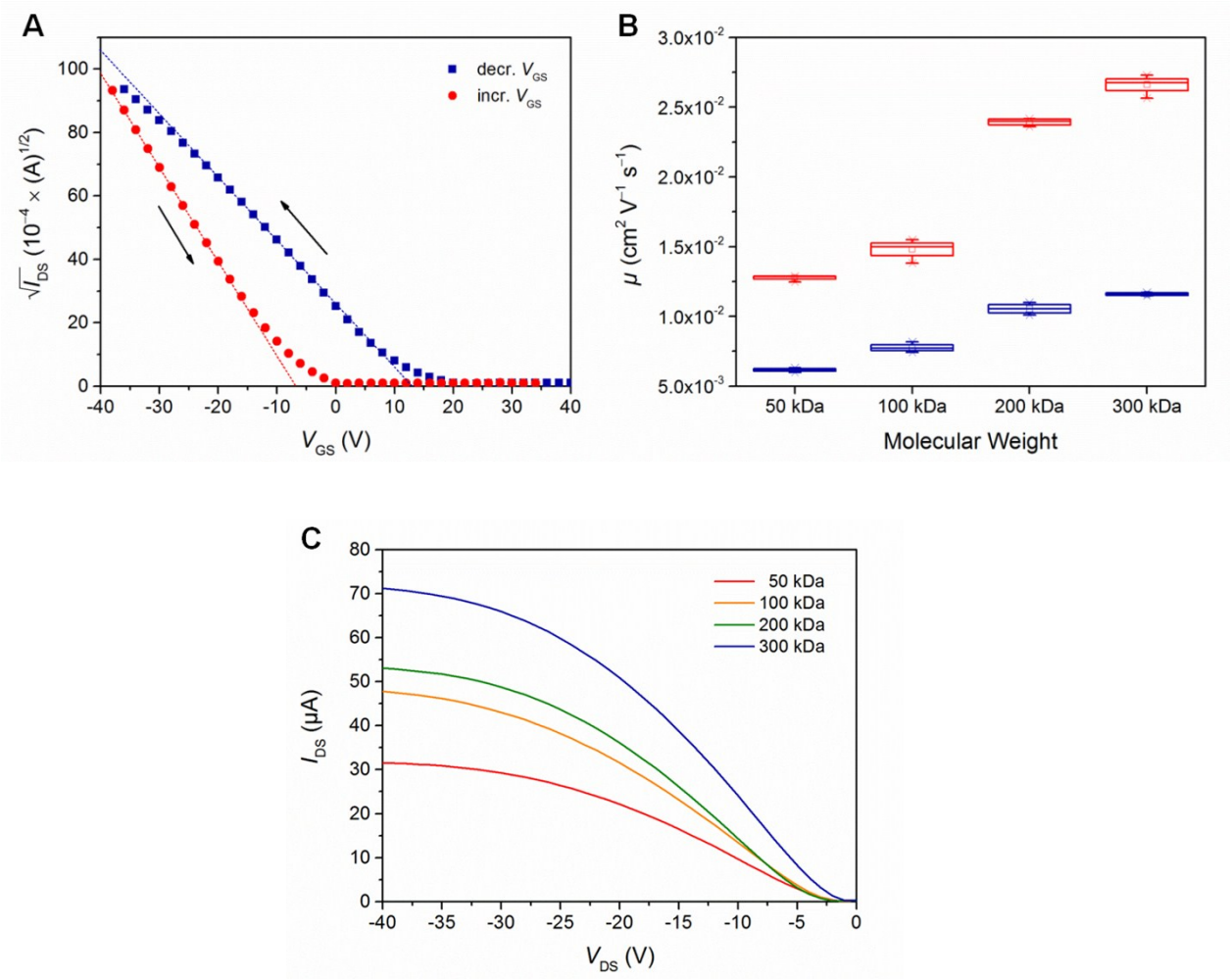

Figure S5. (A) A typical transconductance measurement of a PTB7-Th thin film (200 kDa) using a V_{DS} of −40 V. Squares represent a decreasing V_{GS} sweep from 40 V to −40 V, while circles represent an increasing V_{GS} sweep from −40 V to 40 V. Dotted lines represent a standard transistor equation of I_{DS}−V_{GS} dependence in the saturation regime. (B) Field-effect hole mobility of PTB7-Th thin films with different molecular weight calculated from the saturation transconductance curves. Box plots represent the field-effect hole mobility values extracted from measurements with an increasing V_{GS} voltage (red) and a decreasing V_{GS} voltage (blue). (C) Typical output characteristics of PTB7-Th thin films with different molecular weight at a V_{GS} of −40 V. The results correspond to 20 μm OFETs.

Details of the calculation of the Arrhenius-type activation energy (E_a)

The symbols in Fig. 3B represent the field-effect mobilities of OFETs as a function of 1000/T, where T is the temperature in K. The dotted lines represent the Arrhenius-type dependence

$$\log(\mu/\mu_0) = -E_a/k_B T \quad (1)$$

where E_a is the activation energy, k_B is the Boltzmann constant, T is the temperature, μ_0 is the field-effect mobility at infinite temperature and μ is the field-effect mobility. The field-effect mobility was calculated using standard field-effect transistor equations from the I_{DS}–V_{GS} graphs in the saturation regime as explained in the experimental section. For temperature-dependent field-effect mobility measurements, the device characteristics were measured by sweeping the temperature from −20 ºC to 60 ºC and back from 50 ºC to −10 ºC using a temperature step of 20 ºC with the device temperature being controlling using a Peltier element.

We note that the logarithm of the measured mobility exhibits a linear dependence on 1/T for temperatures above 20 ºC, as demonstrated in Fig. 3B. Therefore, the mobility dependence on T above 20 ºC was analyzed using Eq.(1). Hence, the activation energy (E_a) was estimated using the least-square minimization method of the difference between the logarithm of the measured mobility and the right side of Eq.(1), as presented in Fig. 3B. Consequently, μ_0 and E_a were estimated as the »best-fit« parameters of the Eq.(1) for the temperature above 20 ºC. The values of the model parameters are summarized in Table S2.

Table S2. Values for μ_0 and E_a determined as described above

Molecular Weight	μ_0 [cm^2 V^{-1} s^{-1}]	E_a [meV]
50 kDa	1.7±0.4	165±6
100 kDa	1.6±0.8	156±11
200 kDa	0.29±0.03	98±2
300 kDa	1.8±0.5	142±7

Grazing Incidence X-Ray Diffraction

Table S3. X-ray diffraction peak positions of the (010) reflection and the corresponding *d*-spacing distances for PTB7-Th with different molecular weights deposited from *ortho*-dichlorobenzene solutions via spin coating

Molecular Weight	2θ [deg]	*d* [Å]
50 kDa	22.12	4.02
100 kDa	22.43	3.96
200 kDa	22.06	4.03
300 kDa	22.12	4.02

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