Supplementary information for

Thermal behavior and polymorphism of 2,9-didecyldinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]thiophene thin films

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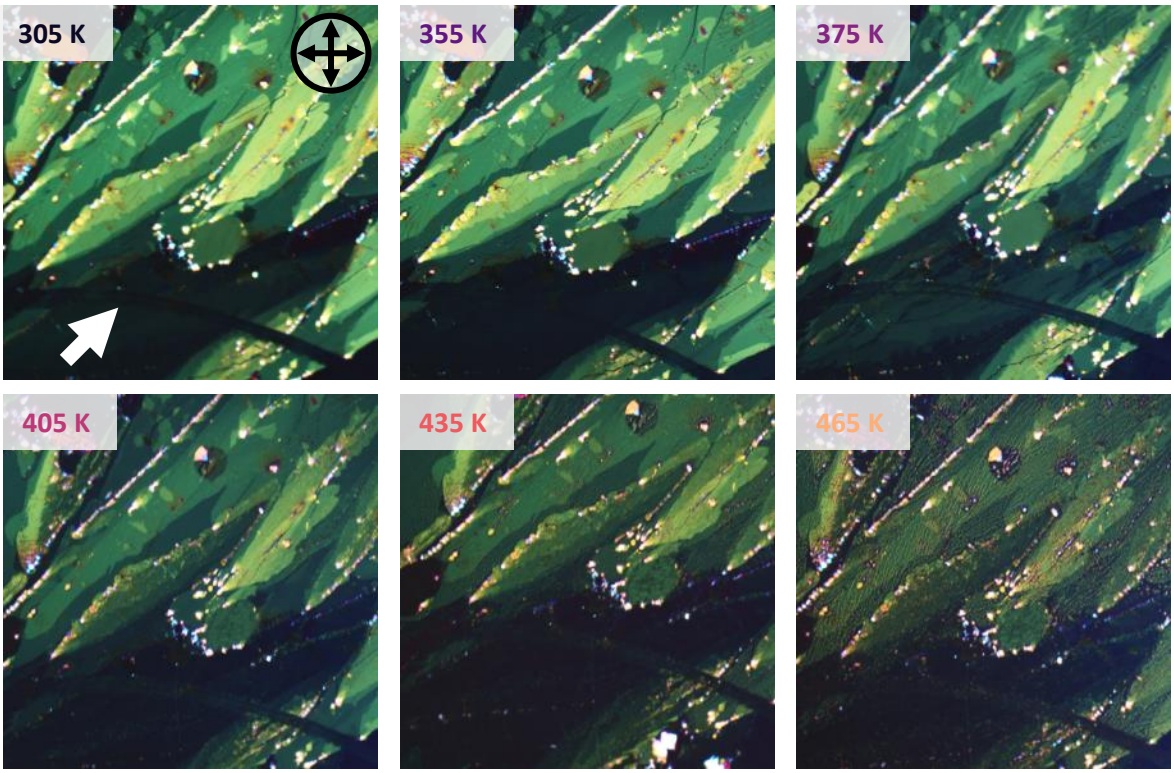

Figure S1: Cross-polarized optical microscopy images of shear-coated C10-DNTT thin films during heating. The images show the same area as in Figure 1, but rotated by 45°. The orange ribbons from Figure 1 are visible here as green ribbons, which do not change their color upon heating. The shear-coating is indicated by the white arrow. The scale bar corresponds to 400 µm.

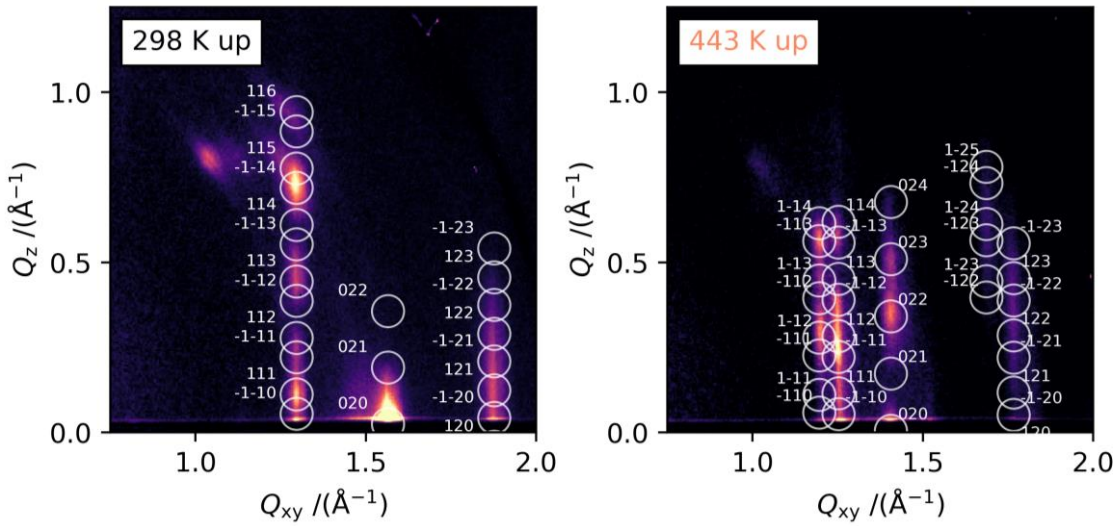

Figure S2: Indexed 2D diffraction patterns at room temperature and at 443 K for the low temperature polymorph Ib and the high temperature polymorph II. The crystal structure refinement for polymorph Ib and II was performed on the respective low and high temperature images. The peak indexing and extraction of the unit cell parameters was performed by using the software WxDiff [47], with the assumption that the a and b axis are parallel to the substrate plane. First the in-plane unit cell parameters a and b were calculated by extracting the Q_{xy} values of the Bragg rods and minimizing the residual between the measured Q_{xy} values and the calculated values $Q_{xy} = \sqrt{\left(ha_{\parallel}^{*} + kb_{\parallel}^{*}\right)^2}$ where hkl are the Miller indices of the reflections and $a_{\parallel}^{*}$, $b_{\parallel}^{*}$ are the reciprocal lattice vectors parallel to the substrate plane. In a next step, the out-of-plane positions of the peaks

are taken into account as well. The Q_z values of a specific reflection can be calculated by $Q_z = (ha_\perp^* + kb_\perp^* + lc^*)$, where hkl are again the Miller indices and $a_\perp^*$, $b_\perp^*$, c^* are the reciprocal lattice vectors perpendicular to the substrate plane. The optimized parameters for the in-plane and complete unit cells are calculated by minimizing a residual between the observed and calculated parameters by the method of least squares.

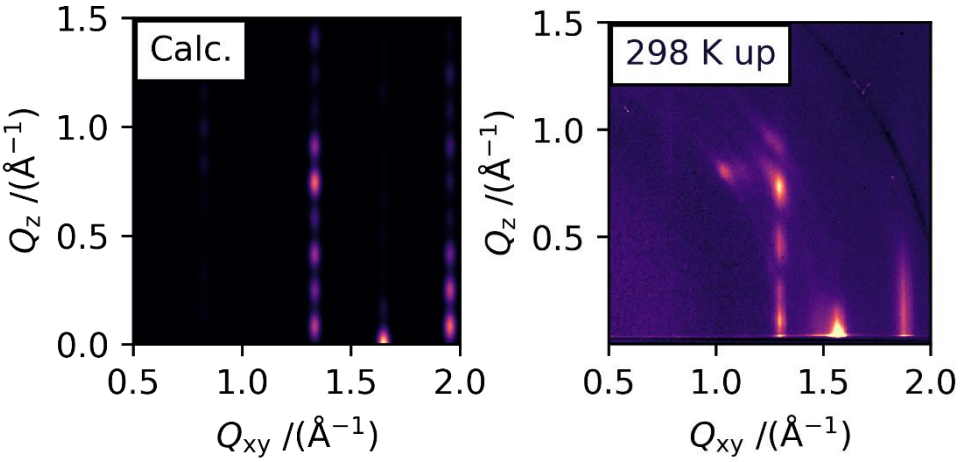

Figure S3: Comparison between 2D diffraction patterns calculated from literature data and the obtained measurement at room temperature. The slight mismatch in in- and out-of-plane scattering vectors is attributed to thermal expansion as the literature data is measured from bulk crystals at 200 K. The Q_{xy} and Q_z values were calculated using the same equations as for the peak indexing and the maximum intensity is calculated from the position of the atoms inside the unit cell. The method for calculating the intensity is the same that is used later in the refinement process and is described in detail in a following section. The full width at half maximum (FWHM) of the peaks is set to 0.04 Å^{-1} in the in-plane direction and 0.1 Å^{-1} in the out-of-plane direction to match the peak widths in the measured diffraction image and to correspond to coherence lengths of 14 nm and 6 nm for the in-plane and out-of-plane direction, respectively. The values were calculated by the Scherrer formula with a K shape factor of 0.9.[48,49]

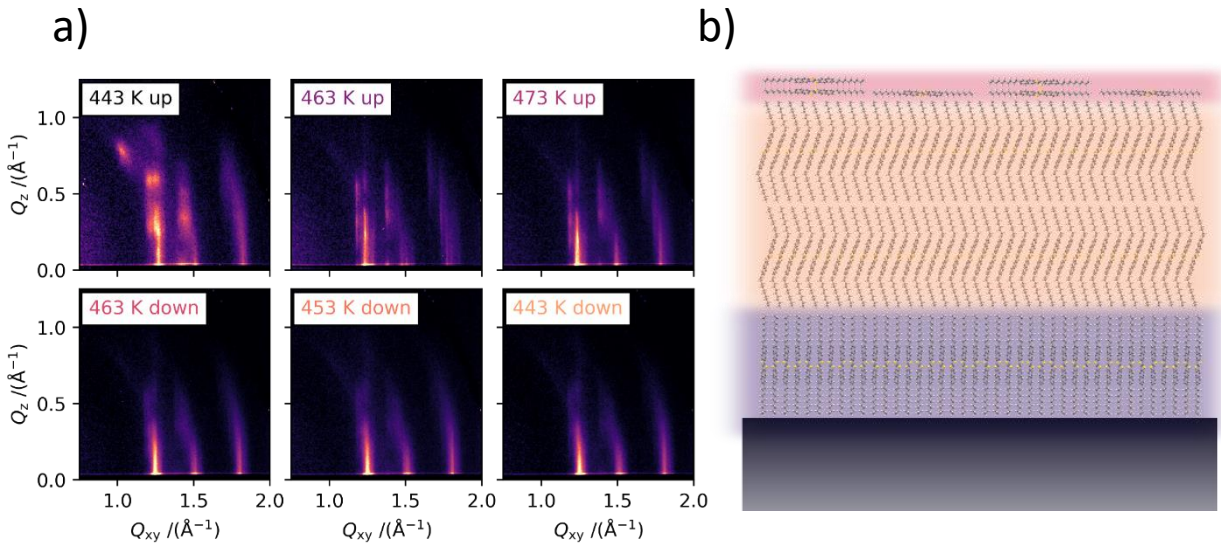

Figure S4: a) GIWAXS images of a sample with extensive beam damage. The intensity of the peaks originating from crystallites in the high temperature polymorph II diminishes and streak-like peaks at the peak positions of the original polymorph Ib reappear. b) Schematic of the film composition. The top layers are comprised of lying molecules, which are removed by the beam damage first. Later the molecules in the high temperature polymorph II (shown with an orange background) are first probed and later destroyed as well. This leaves only the last layer or layers at the bottom of the film left, which resemble the structure of the original polymorph Ib again.

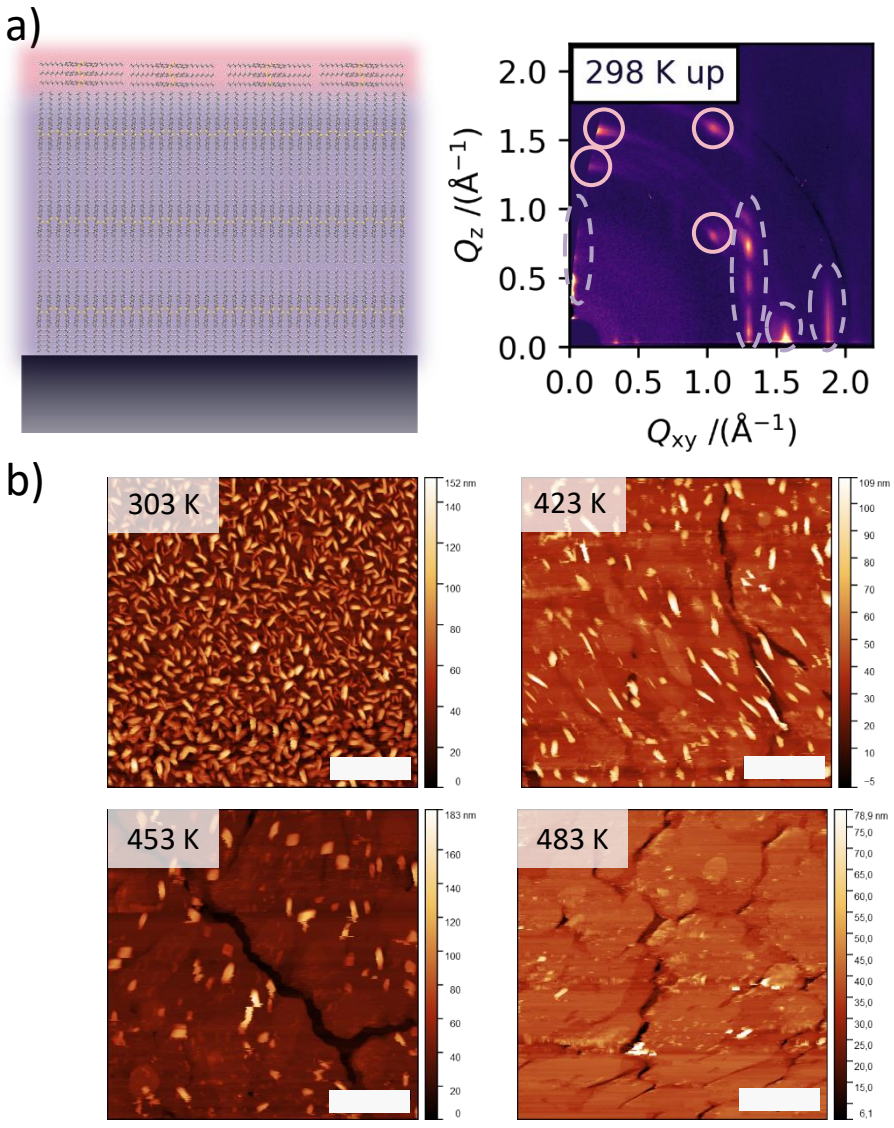

Figure S5: a) Schematic representation of the film structure of evaporated C10-DNTT thin films on the left and a scattering image with highlighted peaks on the right. In the schematic, the layers with the purple background represent standing molecules in the low temperature polymorph Ib and the layers with the red background on top represent molecules in polymorph Ib that are lying on top of the film. In the scattering image, the solid light circles denote peaks originating from the lying molecules on top of the film, whereas the darker dashed circles designate peaks stemming from the film underneath. b) AFM images of evaporated C10-DNTT films after being heated to different temperatures. The reduction of the nanostructures on top of the films at higher temperatures explains the reduction of intensity of the peaks originating from lying crystallites. The scale bar corresponds to 1 µm.

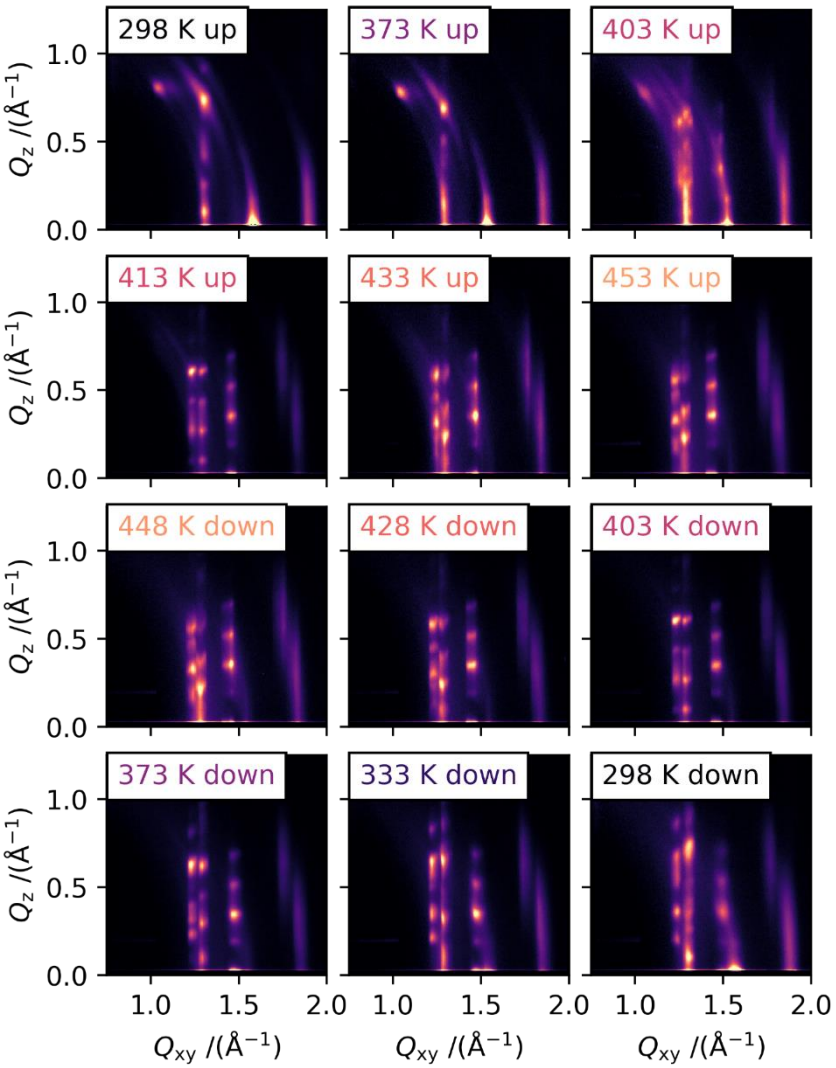

Figure S6: 2D scattering images obtained by GIWAXS measurements at different temperatures of evaporated C10-DNTT thin films with a polystyrene capping layer. A clear change in the diffraction pattern can be observed above 400 K, which persists to over 453 K and during cooling down to room temperature. The observed diffraction patterns of the two polymorphs are equivalent to the ones obtained from films without a capping layer with slightly more defined peaks.

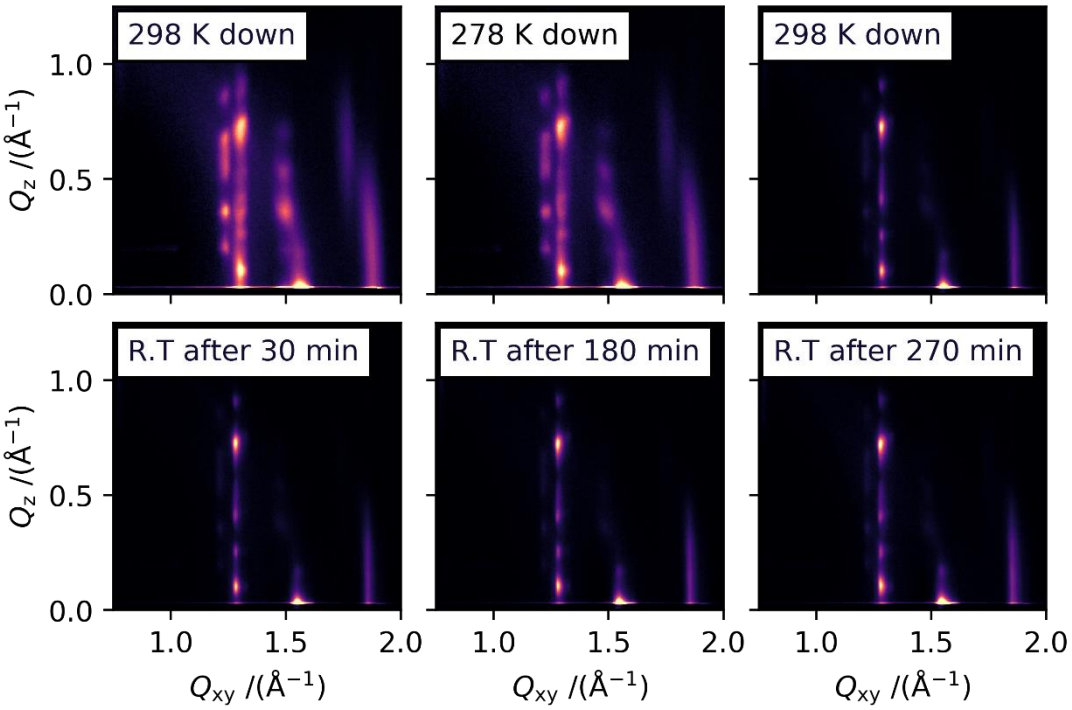

Figure S7: Time series of 2D scattering images obtained by GIWAXS measurements of evaporated C10-DNTT thin films with a polystyrene capping layer after heating and cooling. The scattering intensities of polymorph II are only faintly visible after the films are cooled to 278 K and heated again to room temperature. After this there is no significant change in the diffraction patterns with time.

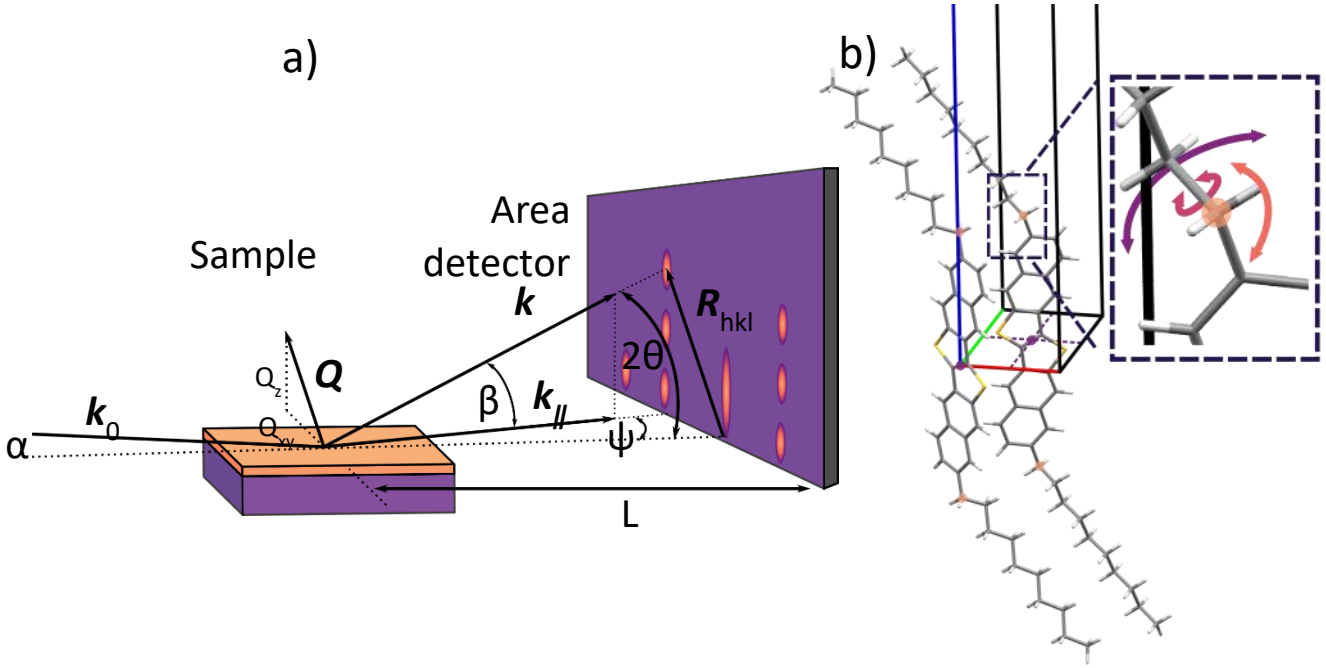

Figure S8: a) Schematic of the GIWAXS setup with the physical quantities used in the equations for the indexing and refinement process. b) Starting position of the molecules for the refinement procedure. The position of the center of mass of the molecules is fixed but rotation in three directions are allowed. The inset shows the possible rotation direction of the ball joint incorporated in the first carbon atom of the alkyl chain.

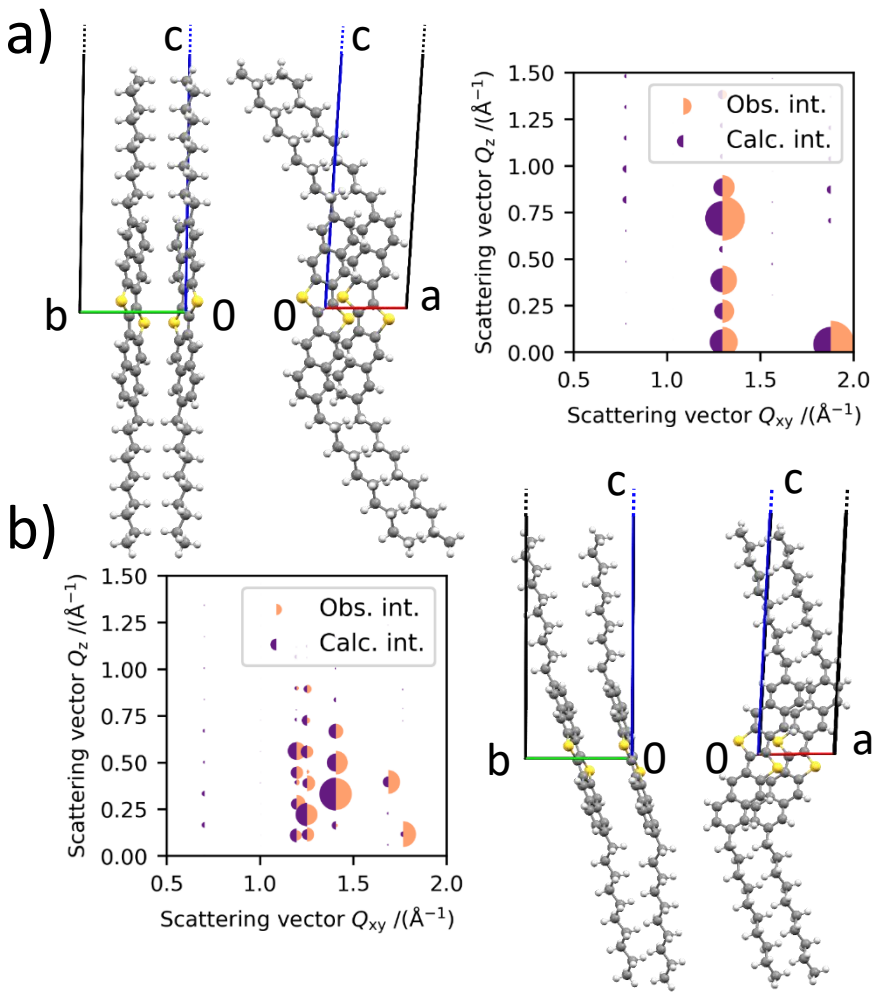

Figure S9: a) Crystal structure of polymorph Ib refined with stiff side chains and the corresponding intensity profiles. The refinement worked well with stiff side chains for the low temperature case, as they are in the same configurations as in the packing obtained from single crystal literature data. b) Crystal structure of polymorph II refined with stiff side chains and the corresponding intensity profiles. The side chains are not completely parallel, which leads to enhanced intensities in the 01l rod (Q_{xy} = 0.7 Å^{-1}) at low Q_z values which are not observed experimentally.

We provide the crystallographic information files (cif) of the low temperature polymorph Ib and the high temperature polymorph II in the following. In order to use them, copy the contents into a file and save it with the .cif extension.

Low temperature polymorph Ib

```
# Disclaimer: This is crystal structure was refined from thin film data
# obtained by GIWAXS measurements and is therefore non-standard.
# The refinement process was heavily constrained. The molecular and
sidechains
# were assumed to be rigid and connected by a 'ball joint'.
# For details please refer to the original publication.
# This cif file contains the low temperature thin film polymorph Ib
# of C10-DNTT.
```

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_chemical_formula_structural       ?
_chemical_melting_point            ?
_chemical_formula_weight           620.96
_symmetry_cell_setting             triclinic

loop_
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_symmetry_equiv_pos_as_xyz
1 x,y,z
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_cell_length_b                          8.0301
_cell_length_c                          37.9349
_cell_angle_alpha                       90.897
_cell_angle_beta                   86.298
_cell_angle_gamma                       90.131
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_diffrn_radiation_type             synchrotron
_diffrn_radiation_wavelength1.0
_diffrn_source                     synchrotron
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loop_
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_atom_site_fract_x
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_atom_site_fract_z
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C     C2    -0.1962     0.0833     0.0923
H     H1    -0.3317     0.1372     0.0990
C     C3    -0.0543     0.0331     0.1182
C     C4    -0.1046     0.0646     0.1546
H     H2    -0.2374     0.1209     0.1618
C     C5    0.0342      0.0159     0.1799
C     C6    0.2294      -0.0709    0.1689
H     H3    0.3233      -0.1083    0.1862
C     C7    0.2860      -0.1022    0.1341
H     H4    0.4199      -0.1588    0.1276
C     C8    0.1479      -0.0517    0.1073
C     C9    0.2047      -0.0797    0.0711
H     H5    0.3380      -0.1355    0.0640
C     C10   0.0666      -0.0258    0.0458
C     C11   0.0890      -0.0332    0.0079
C     C12   -0.0190     0.0583     0.2188
H     H6    -0.0412     0.1802     0.2212
H     H7    0.1105      0.0299     0.2320
```

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H	H9	-0.1935	-0.1495	0.2356
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H	H10	-0.2786	0.1549	0.2745
H	H11	-0.1399	0.0027	0.2880
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H	H12	-0.6006	-0.0136	0.2785
H	H13	-0.4598	-0.1618	0.2934
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H	H14	-0.5302	0.1521	0.3291
H	H15	-0.3933	0.0021	0.3441
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H	H16	-0.8543	-0.0106	0.3352
H	H17	-0.7164	-0.1586	0.3508
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H	H18	-0.6405	0.0134	0.4001
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H	H21	-0.9639	-0.1514	0.4078
C	C20	-1.0150	0.0461	0.4431
H	H22	-1.0308	0.1682	0.4414
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H	H24	-1.2007	-0.1437	0.4652
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H	H26	-1.3467	0.0000	0.4497
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C	C23	0.1962	-0.0833	-0.0923
H	H27	0.3317	-0.1372	-0.0990
C	C24	0.0543	-0.0331	-0.1182
C	C25	0.1046	-0.0646	-0.1546
H	H28	0.2374	-0.1209	-0.1618
C	C26	-0.0342	-0.0159	-0.1799
C	C27	-0.2294	0.0709	-0.1689
H	H29	-0.3233	0.1083	-0.1862
C	C28	-0.2860	0.1022	-0.1341
H	H30	-0.4199	0.1588	-0.1276
C	C29	-0.1479	0.0517	-0.1073
C	C30	-0.2047	0.0797	-0.0711
H	H31	-0.3380	0.1355	-0.0640
C	C31	-0.0666	0.0258	-0.0458
C	C32	-0.0890	0.0332	-0.0079
C	C33	0.0190	-0.0583	-0.2188
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H	H33	-0.1105	-0.0299	-0.2320
C	C34	0.2186	0.0277	-0.2360
H	H34	0.3481	0.0052	-0.2223
H	H35	0.1935	0.1495	-0.2356
C	C35	0.2666	-0.0319	-0.2742
H	H36	0.2786	-0.1549	-0.2745
H	H37	0.1399	-0.0027	-0.2880
C	C36	0.4738	0.0391	-0.2925
H	H38	0.6006	0.0136	-0.2785
H	H39	0.4598	0.1618	-0.2934
C	C37	0.5200	-0.0293	-0.3301
H	H40	0.5302	-0.1521	-0.3291

H	H41	0.3933	-0.0021	-0.3441
C	C38	0.7271	0.0360	-0.3492
H	H42	0.8543	0.0106	-0.3352
H	H43	0.7164	0.1586	-0.3508
C	C39	0.7690	-0.0375	-0.3863
H	H44	0.6405	-0.0134	-0.4001
H	H45	0.7813	-0.1600	-0.3846
C	C40	0.9760	0.0289	-0.4061
H	H46	1.1046	0.0047	-0.3923
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C	C46	0.6086	0.5719	-0.1539
H	H54	0.7422	0.6277	-0.1606
C	C47	0.4697	0.5253	-0.1798
C	C48	0.2731	0.4392	-0.1696
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C	C49	0.2155	0.4064	-0.1352
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H     H96   -0.1396    0.4776     0.4003
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H     H101  -0.3832    0.4692     0.4570
C     C84   -0.7124    0.5247     0.4638
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H     H103  -0.7323    0.4709     0.4867
H     H104  -0.8438    0.5063     0.4505
###------------------------------------------ End of content of .cif
file -------------------------------
```

High temperature polymorph II

```
# Disclaimer: This is crystal structure was refined from thin film data
# obtained by GIWAXS measurements and is therefore non-standard.
# The refinement process was heavily constrained. The molecular and
sidechains
# were assumed to be rigid and connected by a 'ball joint'.
# For details please refer to the original publication.
# This cif file contains the high temperature thin film polymorph II
# of C10-DNTT.

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_cell_length_c                          37.4332
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_cell_angle_gamma                       92.811
_cell_volume                            2096.276
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_cell_measurement_temperature      443
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_exptl_crystal_colour              yellow
_diffrn_ambient_temperature        293
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_diffrn_radiation_type             synchrotron
_diffrn_radiation_wavelength1.0
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loop_
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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
S     S1    0.2927      -0.0455     -0.0271
C     C1    0.1378      0.0415      -0.0581
C     C2    0.2035      0.0757      -0.0925
H     H1    0.3422      0.0521      -0.1016
C     C3    0.0631      0.1470      -0.1145
C     C4    0.1246      0.1889      -0.1500
H     H2    0.2639      0.1685      -0.1594
C     C5    -0.0123     0.2587      -0.1715
C     C6    -0.2210     0.2856      -0.1574
H     H3    -0.3179     0.3303      -0.1722
```

C	C7	-0.2864	0.2488	-0.1231
H	H4	-0.4266	0.2705	-0.1144
C	C8	-0.1482	0.1785	-0.1001
C	C9	-0.2105	0.1420	-0.0644
H	H5	-0.3497	0.1628	-0.0550
C	C10	-0.0692	0.0757	-0.0428
C	C11	-0.0894	0.0326	-0.0057
C	C12	0.0615	0.3090	-0.2091
H	H6	-0.0709	0.3331	-0.2207
H	H7	0.0468	0.2025	-0.2021
C	C13	0.2470	0.3284	-0.2365
H	H8	0.2684	0.4356	-0.2429
H	H9	0.3787	0.2968	-0.2260
C	C14	0.2088	0.2371	-0.2704
H	H10	0.0705	0.2636	-0.2795
H	H11	0.1966	0.1298	-0.2640
C	C15	0.3803	0.2590	-0.3003
H	H12	0.3969	0.3667	-0.3063
H	H13	0.5179	0.2281	-0.2917
C	C16	0.3310	0.1703	-0.3341
H	H14	0.1916	0.2000	-0.3422
H	H15	0.3163	0.0626	-0.3280
C	C17	0.4961	0.1908	-0.3648
H	H16	0.5130	0.2985	-0.3709
H	H17	0.6352	0.1590	-0.3571
C	C18	0.4389	0.1027	-0.3982
H	H18	0.4199	-0.0046	-0.3919
H	H19	0.3006	0.1357	-0.4060
C	C19	0.6053	0.1206	-0.4293
H	H20	0.6243	0.2280	-0.4356
H	H21	0.7438	0.0877	-0.4215
C	C20	0.5454	0.0315	-0.4624
H	H22	0.4087	0.0661	-0.4705
H	H23	0.5232	-0.0755	-0.4560
C	C21	0.7129	0.0469	-0.4927
H	H24	0.8477	0.0102	-0.4851
H	H25	0.6662	-0.0119	-0.5133
H	H26	0.7339	0.1524	-0.4995
S	S2	-0.2927	0.0455	0.0271
C	C22	-0.1378	-0.0415	0.0581
C	C23	-0.2035	-0.0757	0.0925
H	H27	-0.3422	-0.0521	0.1016
C	C24	-0.0631	-0.1470	0.1145
C	C25	-0.1246	-0.1889	0.1500
H	H28	-0.2639	-0.1685	0.1594
C	C26	0.0123	-0.2587	0.1715
C	C27	0.2210	-0.2856	0.1574
H	H29	0.3179	-0.3303	0.1722
C	C28	0.2864	-0.2488	0.1231
H	H30	0.4266	-0.2705	0.1144
C	C29	0.1482	-0.1785	0.1001
C	C30	0.2105	-0.1420	0.0644
H	H31	0.3497	-0.1628	0.0550
C	C31	0.0692	-0.0757	0.0428
C	C32	0.0894	-0.0326	0.0057
C	C33	-0.0615	-0.3090	0.2091
H	H32	0.0709	-0.3331	0.2207
H	H33	-0.0468	-0.2025	0.2021
C	C34	-0.2470	-0.3284	0.2365

H	H34	-0.2684	-0.4356	0.2429
H	H35	-0.3787	-0.2968	0.2260
C	C35	-0.2088	-0.2371	0.2704
H	H36	-0.0705	-0.2636	0.2795
H	H37	-0.1966	-0.1298	0.2640
C	C36	-0.3803	-0.2590	0.3003
H	H38	-0.3969	-0.3667	0.3063
H	H39	-0.5179	-0.2281	0.2917
C	C37	-0.3310	-0.1703	0.3341
H	H40	-0.1916	-0.2000	0.3422
H	H41	-0.3163	-0.0626	0.3280
C	C38	-0.4961	-0.1908	0.3648
H	H42	-0.5130	-0.2985	0.3709
H	H43	-0.6352	-0.1590	0.3571
C	C39	-0.4389	-0.1027	0.3982
H	H44	-0.4199	0.0046	0.3919
H	H45	-0.3006	-0.1357	0.4060
C	C40	-0.6053	-0.1206	0.4293
H	H46	-0.6243	-0.2280	0.4356
H	H47	-0.7438	-0.0877	0.4215
C	C41	-0.5454	-0.0315	0.4624
H	H48	-0.4087	-0.0661	0.4705
H	H49	-0.5232	0.0755	0.4560
C	C42	-0.7129	-0.0469	0.4927
H	H50	-0.8477	-0.0102	0.4851
H	H51	-0.6662	0.0119	0.5133
H	H52	-0.7339	-0.1524	0.4995
S	S3	0.2068	0.3825	0.0125
C	C43	0.3603	0.3718	0.0504
C	C44	0.2934	0.3039	0.0817
H	H53	0.1546	0.2567	0.0845
C	C45	0.4328	0.3046	0.1102
C	C46	0.3700	0.2397	0.1436
H	H54	0.2306	0.1941	0.1471
C	C47	0.5060	0.2405	0.1715
C	C48	0.7149	0.3059	0.1657
H	H55	0.8111	0.3040	0.1844
C	C49	0.7815	0.3716	0.1340
H	H56	0.9218	0.4164	0.1312
C	C50	0.6443	0.3743	0.1050
C	C51	0.7078	0.4441	0.0722
H	H57	0.8472	0.4898	0.0688
C	C52	0.5675	0.4460	0.0448
C	C53	0.5891	0.5128	0.0098
C	C54	0.4308	0.1758	0.2078
H	H58	0.4920	0.2800	0.2067
H	H59	0.5414	0.1124	0.2166
C	C55	0.2420	0.1700	0.2348
H	H60	0.1268	0.2287	0.2257
H	H61	0.1864	0.0651	0.2376
C	C56	0.3027	0.2323	0.2712
H	H62	0.3694	0.3340	0.2676
H	H63	0.4114	0.1689	0.2806
C	C57	0.1188	0.2407	0.2990
H	H64	0.0072	0.3011	0.2893
H	H65	0.0556	0.1387	0.3035
C	C58	0.1853	0.3094	0.3344
H	H66	0.2516	0.4105	0.3296
H	H67	0.2958	0.2479	0.3440

C	C59	0.0063	0.3224	0.3627
H	H68	-0.1057	0.3828	0.3531
H	H69	-0.0583	0.2214	0.3681
C	C60	0.0788	0.3939	0.3973
H	H70	0.1922	0.3341	0.4066
H	H71	0.1417	0.4954	0.3919
C	C61	-0.0996	0.4059	0.4263
H	H72	-0.2131	0.4659	0.4171
H	H73	-0.1628	0.3045	0.4318
C	C62	-0.0240	0.4776	0.4608
H	H74	0.0360	0.5800	0.4555
H	H75	0.0918	0.4190	0.4697
C	C63	-0.1999	0.4859	0.4896
H	H76	-0.2574	0.3847	0.4955
H	H77	-0.1430	0.5331	0.5110
H	H78	-0.3141	0.5452	0.4811
S	S4	0.7932	0.6175	-0.0125
C	C64	0.6397	0.6282	-0.0504
C	C65	0.7066	0.6961	-0.0817
H	H79	0.8454	0.7433	-0.0845
C	C66	0.5672	0.6954	-0.1102
C	C67	0.6300	0.7603	-0.1436
H	H80	0.7694	0.8059	-0.1471
C	C68	0.4940	0.7595	-0.1715
C	C69	0.2851	0.6941	-0.1657
H	H81	0.1889	0.6960	-0.1844
C	C70	0.2185	0.6284	-0.1340
H	H82	0.0782	0.5836	-0.1312
C	C71	0.3557	0.6257	-0.1050
C	C72	0.2922	0.5559	-0.0722
H	H83	0.1528	0.5102	-0.0688
C	C73	0.4325	0.5540	-0.0448
C	C74	0.4109	0.4872	-0.0098
C	C75	0.5692	0.8242	-0.2078
H	H84	0.5080	0.7200	-0.2067
H	H85	0.4586	0.8876	-0.2166
C	C76	0.7580	0.8300	-0.2348
H	H86	0.8732	0.7713	-0.2257
H	H87	0.8136	0.9349	-0.2376
C	C77	0.6973	0.7677	-0.2712
H	H88	0.6306	0.6660	-0.2676
H	H89	0.5886	0.8311	-0.2806
C	C78	0.8812	0.7593	-0.2990
H	H90	0.9928	0.6989	-0.2893
H	H91	0.9444	0.8613	-0.3035
C	C79	0.8147	0.6906	-0.3344
H	H92	0.7484	0.5895	-0.3296
H	H93	0.7042	0.7521	-0.3440
C	C80	0.9937	0.6776	-0.3627
H	H94	1.1057	0.6172	-0.3531
H	H95	1.0583	0.7786	-0.3681
C	C81	0.9212	0.6061	-0.3973
H	H96	0.8078	0.6659	-0.4066
H	H97	0.8583	0.5046	-0.3919
C	C82	1.0996	0.5941	-0.4263
H	H98	1.2131	0.5341	-0.4171
H	H99	1.1628	0.6955	-0.4318
C	C83	1.0240	0.5224	-0.4608
H	H100	0.9640	0.4200	-0.4555

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H     H101  0.9082     0.5810     -0.4697
C     C84   1.1999     0.5141     -0.4896
H     H102  1.2574     0.6153     -0.4955
H     H103  1.1430     0.4669     -0.5110
H     H104  1.3141     0.4548     -0.4811
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References

(47) S. C. B. Mannsfeld, WxDiff, Stanford Synchrotron Radiation Lightsource, 2009

(48) B. E. Warren, X-Ray Diffraction, Addison-Wesley Pub. Co.: Reading, Mass., 1969

(49) Rivnay J., Mannsfeld S. C. B., Miller C. E., Salleo A., Toney M. F., Quantitative Determination of Organic Semiconductor Microstructure from the Molecular to Device Scale *Chem. Rev.,* 2012, **112**, 10, 5488-5519, DOI: 10.1021/cr3001109.