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Dipolar Guest Orientation in Polymer Co-crystals and Macroscopic Films

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Electronic Supplementary Information: Tables containing the fractional coordinates of the models presented in the manuscript and the structure factors (calculated and observed).

Table 1. Fractional coordinates of the atoms of the asymmetric unit of the model presented in Figure 4 of the manuscript for the s-PS/NB δ clathrate form according the space group $P2_1/a$. Hydrogen atoms were included in the structure factors calculation, but they are omitted in this Table for simplicity.

s-PS/NB			
	x/a	y/b	z/c
C1	0.251	-0.004	0.507
C2	0.273	-0.075	0.634
C3	0.160	-0.001	0.255
C4	0.175	-0.079	0.379
C5	0.090	-0.163	0.472
C6	0.049	-0.120	0.575
C7	-0.031	-0.198	0.655
C8	-0.071	-0.321	0.632
C9	-0.031	-0.365	0.531
C10	0.049	-0.286	0.452
C11	0.297	-0.153	0.534
C12	0.366	-0.105	0.419
C13	0.386	-0.178	0.326
C14	0.337	-0.302	0.349
C15	0.268	-0.351	0.467
C16	0.249	-0.276	0.558
C17	0.412	0.503	0.522
C18	0.519	0.409	0.512
C19	0.375	0.379	0.523
C20	0.557	0.533	0.511
C21	0.428	0.333	0.517
C22	0.503	0.581	0.516
N1	0.651	0.612	0.506
O1	0.695	0.566	0.506
O2	0.682	0.718	0.504

Table 2. Structure factors calculated (F_{calcd}) according the space group $P2_1/a$ imposing an occupancy factor for the guest molecules of 0.9, for the model of the δ co-crystalline form of s-PS with nitrobenzene reported in Figure 4 of the manuscript. Observed structure factors (F_{obsd}), as evaluated from the intensities of the reflections of the X-ray fiber diffraction pattern of Figure 2 (A). The Bragg distances (d_{obsd}), observed in the X-ray fiber diffraction pattern and calculated (d_{calcd}) for the proposed monoclinic unit cell (a = 1.80 nm, b = 1.32 nm, c = 0.78 nm and γ= 107.8°), are also shown. Reflections not observed with F_{calcd} less than 25 have not been reported.

hkl	d_{calcd} (nm)	d_{obsd} (nm)	F_{calcd}	F_{obsd}
010	1.12	1.12	45	57
$2\bar{1}0$	0.89	0.86	57	83
200	0.76	-	27	-
$2\bar{2}0$	0.64	-	27	-
020	0.56	0.56	16	22
210	0.52	0.51	74	58
$4\bar{2}0$ $2\bar{3}0$ $4\bar{1}0$	0.44 0.44 0.44	0.44	41 66 25 } 82	79
$4\bar{3}0$ 400 030 220	0.39 0.38 0.37 0.37	0.38	37 19 48 42 } 76	71
$2\bar{4}0$	0.32	-	26	22
040	0.28	0.29	38	20
$6\bar{4}0$	0.27	-	27	-
$4\bar{5}0$	0.26	0.26	24	-
$1\bar{1}1$ 011	0.67 0.64	0.66	24 2 } 24	31
201 111 $1\bar{2}1$ $2\bar{2}1$	0.55 0.54 0.50 0.50	0.52	18 103 112 34 } 157	177
$3\bar{1}1$	0.47	-	25	-
021 $3\bar{2}1$ 211 301	0.46 0.45 0.43 0.43	0.44	3 106 28 94 } 144	152
$4\bar{2}1$ $2\bar{3}1$ $4\bar{1}1$ $3\bar{3}1$	0.39 0.38 0.38 0.38	0.38	89 28 94 15 } 133	97
311	0.35	-	26	-
$1\bar{4}1$	0.28	-	28	-
501	0.28	-	26	-
$6\bar{4}1$	0.26	-	28	-

$\left\{\begin{matrix}102\\ 1\bar{1}2\\ 012\\ 2\bar{1}2\\ 202\\ 112\end{matrix}\right.$	$\begin{matrix}0.38\\ 0.37\\ 0.37\\ 0.36\\ 0.35\\ 0.34\end{matrix}$	0.36	$\left.\begin{matrix}32\\ 50\\ 59\\ 72\\ 5\\ 38\end{matrix}\right\}117$	138
$2\bar{2}2$	0.33	-	26	-
$\left\{\begin{matrix}3\bar{1}2\\ 022\\ 3\bar{2}2\\ 212\\ 302\end{matrix}\right.$	$\begin{matrix}0.33\\ 0.32\\ 0.32\\ 0.31\\ 0.31\end{matrix}$	0.32	$\left.\begin{matrix}12\\ 1\\ 59\\ 23\\ 61\end{matrix}\right\}81$	89
$4\bar{2}2$	0.29	-	40	-
$\left\{\begin{matrix}312\\ 4\bar{3}2\\ 402\\ 032\end{matrix}\right.$	$\begin{matrix}0.28\\ 0.28\\ 0.27\\ 0.27\end{matrix}$	0.27	$\left.\begin{matrix}12\\ 50\\ 47\\ 15\end{matrix}\right\}72$	51
$5\bar{1}2$	0.26	-	25	-
$5\bar{3}2$	0.26	-	32	-

Table 3. Fractional coordinates of the atoms of an asymmetric unit of the minimum energy model found for the δ co-crystalline form s-PS/NA according the space group $P2_1/a$.

	s-PS/NA		
	x/a	*y/b*	*z/c*
C1	0.243	-0.007	0.501
C2	0.039	-0.302	0.451
C3	0.297	-0.151	0.519
C4	0.366	-0.096	0.401
C5	0.390	-0.166	0.308
C6	0.344	-0.294	0.332
C7	0.275	-0.350	0.451
C8	0.252	-0.278	0.543
C9	0.270	-0.076	0.623
C10	0.153	-0.010	0.242
C11	0.168	-0.088	0.371
C12	0.082	-0.173	0.464
C13	0.041	-0.127	0.561
C14	-0.040	-0.205	0.642
C15	-0.082	-0.333	0.626
C16	-0.042	-0.382	0.531
C17	0.563	0.457	0.482
C18	0.470	0.573	0.502
C19	0.610	0.587	0.490
C20	0.424	0.443	0.493
C21	0.562	0.644	0.501
C22	0.471	0.385	0.484
N1	0.703	0.659	0.485
N2	0.328	0.370	0.492
O1	0.291	0.426	0.497
O2	0.291	0.259	0.484

Table 4. Fractional coordinates of the atoms of an asymmetric unit of the triclinic model of the Figure 7 of the manuscript (unit cell parameters: a = 1.795 nm, b = 1.29 nm, c = 0.78 nm, α = 98°, β = 90° and γ = 122.3°) for the δ co-crystalline form s-PS/NA according the space group $\overline{P}1$. Hydrogen atoms were included in the structure factors calculation, but they are omitted in this Table for simplicity

	s-PS/NA		
	x/a	*y/b*	*z/c*
C1	0.247	-0.278	0.481
C2	0.287	-0.345	0.380
C3	0.395	-0.159	0.276
C4	0.366	-0.093	0.379
C5	0.356	-0.286	0.276
C6	0.044	-0.296	0.415
C7	-0.032	-0.374	0.490
C8	-0.074	-0.324	0.589
C9	-0.038	-0.196	0.613
C10	0.039	-0.120	0.536
C11	0.081	-0.168	0.435
C12	0.165	-0.086	0.351
C13	0.342	0.006	0.743
C14	0.266	-0.079	0.600
C15	0.296	-0.151	0.483
C16	0.242	-0.006	0.494
C17	0.578	0.338	1.180
C18	0.224	0.076	1.136
C19	0.148	-0.009	0.241
C20	0.536	0.210	1.180
C21	0.324	0.083	0.887
C22	0.411	0.172	0.998
C23	0.453	0.299	1.003
C24	0.122	0.093	0.932
C25	0.098	0.163	0.852
C26	0.151	0.292	0.886
C27	0.226	0.351	1.003
C28	0.249	0.003	0.999
C29	0.453	0.129	1.089
C30	0.536	0.382	1.093
C31	0.197	0.150	1.048
C32	0.249	0.280	1.082
C33	-0.033	0.568	0.964
C34	0.599	0.500	0.542
C35	0.634	0.611	0.474
C36	0.576	0.647	0.429
C37	0.509	0.426	0.562
C38	0.486	0.574	0.449
C39	0.082	0.499	1.060
C40	0.115	0.604	0.978
C41	-0.064	0.464	1.047
C42	0.452	0.462	0.514
C43	-0.006	0.429	1.093
C44	0.055	0.636	0.930
N1	-0.156	0.394	1.087
N2	0.358	0.387	0.535
N3	0.204	0.675	0.949
N4	0.724	0.683	0.451
O1	0.311	0.419	0.484
O2	0.332	0.295	0.602
O3	-0.180	0.303	1.154
O4	-0.202	0.433	1.054

Table 5. Structure factors calculated (F_{calcd}) according the space group $\overline{P}1$, for the model of the δ co-crystalline form of s-PS 4-nitroaniline presented in Figure 7 of the manuscript. Observed structure factors (F_{obsd}), as evaluated from the intensities of the reflections of the X-ray fiber diffraction pattern of Figure 2(B). The Bragg distances (d_{obsd}), observed in the X-ray fiber diffraction pattern and calculated (d_{calcd}) for the proposed triclinic unit cell (a = 1.795 nm, b = 1.29 nm, c = 0.78 nm, α = 98°, β = 90° and γ= 122.3°), are also shown. Reflections not observed with F_{calcd} less than 25 have not been reported.

hkl	d_{calcd} (nm)	d_{obsd} (nm)	F_{calcd}	F_{obsd}
010	1.08	1.07	41	47
$2\bar{1}0$	0.88	0.87	42	50
$3\bar{2}0$	0.54	0.54	2	19
020	0.54		9 } 10	
300	0.50	0.51	7	44
210	0.50		64 } 64	
$4\bar{2}0$	0.44	0.44	32	65
$4\bar{1}0$	0.44		16	
120	0.44		4 } 73	
$2\bar{3}0$	0.42		63	
310	0.38	0.39	2	34
$4\bar{3}0$	0.38		27 } 30	
400	0.38		13	
030	0.36	-	40	-
220	0.36	-	25	-
$10\bar{1}$	0.71	0.65	1	53
$1\bar{1}1$	0.69		9	
$01\bar{1}$	0.68		8 } 42	
101	0.66		25	
$1\bar{1}\bar{1}$	0.62		32	
011	0.58	Broad: centered at 0.53	9	173
$2\bar{1}\bar{1}$	0.57		6	
$11\bar{1}$	0.57		70	
$20\bar{1}$	0.56		4	
$1\bar{2}1$	0.53		103 } 153	
201	0.52		15	
$2\bar{2}1$	0.52		30	
111	0.49		81	
$3\bar{1}\bar{1}$	0.47	Broad: centered at 0.44	24	180
$3\bar{1}1$	0.47		48	
$22\bar{1}$	0.46		33	
$3\bar{2}1$	0.46		77	
$1\bar{2}\bar{1}$	0.45		101	
$21\bar{1}$	0.45		25	
$30\bar{1}$	0.44		85 } 198	
$3\bar{2}\bar{1}$	0.43		70	
$02\bar{1}$	0.41		17	
121	0.41		26	
301	0.41		71	
211	0.40		23	
$4\bar{2}1$	0.39	0.38	79	128
$4\bar{1}\bar{1}$	0.39		84	
$3\bar{3}1$	0.39		7	
$1\bar{3}1$	0.38		14 } 141	
$4\bar{2}\bar{1}$	0.38		52	
$4\bar{1}1$	0.37		59	
$31\bar{1}$	0.36		5	
$3\bar{3}\bar{1}$	0.35	-	29	-
102	0.37	0.36	51	96
$11\bar{2}$	0.36		40	
$2\bar{1}2$	0.36		54	
$1\bar{1}\bar{2}$	0.36		55 } 115	
$20\bar{2}$	0.36		30	
$1\bar{2}2$	0.35		29	
$2\bar{1}\bar{2}$	0.35		35	
012	0.34	-	69	-
$3\bar{1}2$	0.33	0.32	16	98
$3\bar{2}2$	0.32		28	
$3\bar{1}2$	0.32		27	
$30\bar{2}$	0.32		42	
112	0.32		5	
$12\bar{2}$	0.32		3	
$2\bar{2}\bar{2}$	0.31		34 } 80	
$2\bar{3}2$	0.31		9	
$1\bar{2}\bar{2}$	0.31		4	
$3\bar{2}\bar{2}$	0.31		33	
$1\bar{3}2$	0.30		4	
$3\bar{3}2$	0.30		22	
$4\bar{2}2$	0.29	-	45	-
$4\bar{1}\bar{2}$	0.29	-	44	-
302	0.29	-	39	-
022	0.29	-	28	-
$31\bar{2}$	0.29	-	27	-
$40\bar{2}$	0.28	-	32	-
$4\bar{3}\bar{2}$	0.26	-	36	-
402	0.26	-	40	-