Supplementary information for

Structure and molecular packing in smectic B_{Cr} and A_d phases of Schiff base liquid crystal compounds through the analyses of layer spacing, entropy and crystal structure

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Table S1. Experimental Conditions and Crystallographic Parameters.

	5CBAA
Chemical formula	$C_{18}H_{20}ClNO$
Formula Weight	301.81
Crystal size (mm)	0.34×0.30×0.02
T / K	295(2)
Wavelength / Å	0.71073
Crystal system	Orthorhombic
Space group	$Pca2_1$
a / Å	6.1002(3)
b / Å	7.3335(4)
c / Å	36.4538(18)
V / Å^3	1630.79(14)
Z	4
F(000)	640
Dx / Mg·m^{-3}	1.229
μ / mm^{-1}	0.233
Absorption correction	Numerical (*SADABS*)
T_{max} and T_{min}	1.00, 0.91
θ_{max} / °	27.47
Index ranges	-7 <= h <= 6
	-9 <= k <= 9
	-41 <= l <= 47
No. of .reflections collected	10115
No. of independent reflections	3309 [R(int)=0.0192]
Completeness	99.9% [θ <= 27.47°]
No. of reflections [$I > 2\sigma(I)$]	2553
Refinement method	Full-matrix least-squares on F^2
H-atom parameters	Refined all
No. of data used in refinement	3309
No. of parameters	259
No. of restrainets	1
$R[F^2 > 2\sigma(F^2)]$	0.0389
c_1 and c_2 (*)	0.0584, 0.0894
$wR(F^2)$	0.1128
S	1.083
Absolute structure parameter (**)	-0.04(5)
$(\Delta/\sigma)_{max}$	< 0.001
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e Å^{-3})	0.112, -0.144

(*) $w = 1 / [\sigma^2(F_o^2) + (c_1 \cdot P)^2 + c_2 \cdot P]$ where $P = (F_o^2 + 2F_c^2) / 3$

(**) Flack x determined using 914 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons et al., 2013)

Table S2. Experimental Conditions and Crystallographic Parameters.

	5ABCA	
Chemical formula	$C_{18}H_{20}ClNO$	
Formula Weight	301.81	
	RT phase	LT phase
Crystal size (mm)	0.32×0.18×0.04	0.40×0.26×0.04
T / K	295(2)	106(1)
Wavelength / Å	0.71073	1.5412
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	$P1$-
a / Å	19.3197(6)	18.4072(7)
b / Å	8.6990(2)	8.61246(16)
c / Å	9.8963(3)	9.9664(2)
α / °		93.7782(16)
β / °	92.2801(15)	90.5052(14)
γ / °		95.6436(10)
V / Å^3	1661.88(8)	1568.73(7)
Z	4	4
F(000)	640	640
Dx / Mg·m^{-3}	1.206	1.278
μ / mm^{-1}	0.229	0.213
Absorption correction	Numerical (*SADABS*)	Not performed
T_{max} and T_{min}	0.99, 0.95	
θ_{max} / °	25.37	68.21
Index ranges	-23 <= h <= 23	-22 <= h <= 22
	-10 <= k <= 10	-10 <= k <= 10
	-11 <= l <= 11	-5 <= l <= 5
No. of .reflections collected	40074	6530
No. of independent reflections	3045 [R(int)=0.0234]	2907 [R(int)=0.0314]
Completeness	99.9% [θ <= 25.37°]	50.5% [θ <= 68.21°]
No. of reflections [$I > 2\sigma(I)$]	2155	5573
Refinement method	Full-matrix least-squares on F^2	
H-atom parameters	Mixed	Refined 2-component twin Constrained
No. of data used in refinement	3045	6530
No. of parameters	252	382
No. of restrainets	3	0
$R[F^2 > 2\sigma(F^2)]$	0.0406	0.0786
c_1 and c_2 (*)	0.0460, 0.3384	0.1133, 4.7614
$wR(F^2)$	0.1154	0.2983
S	1.059	1.246
$(\Delta/\sigma)_{max}$	< 0.001	< 0.001
$\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e Å^{-3})	0.158, -0.209	0.378, -0.432

(*) $w = 1 / [\sigma^2(F_o^2) + (c_1 \cdot P)^2 + c_2 \cdot P]$ where $P = (F_o^2 + 2F_c^2) / 3$

Table S3. Standard thermodynamic quantities of 5CBAA.

T / K	C_p / J K^{-1} mol^{-1}	$[H°(T) - H°(0)] / T$ / J K^{-1} mol^{-1}	$S°(T) - S°(0)$ / J K^{-1} mol^{-1}	$-[G°(T) - H°(0)] / T$ / J K^{-1} mol^{-1}
Crystal (K)				
10	6.65	1.76	2.36	0.597
20	25.63	8.72	12.47	3.75
30	47.51	18.00	26.99	9.00
40	67.89	27.97	43.50	15.54
50	86.24	37.82	60.66	22.84
60	102.79	47.29	77.87	30.58
70	117.78	56.31	94.86	38.55
80	131.43	64.86	111.49	46.63
90	143.99	72.96	127.71	54.75
100	155.68	80.65	143.49	62.83
110	166.74	87.98	158.85	70.87
120	177.41	94.99	173.82	78.83
130	187.91	101.74	188.43	86.70
140	198.32	108.26	202.74	94.48
150	208.71	114.61	216.78	102.16
160	219.14	120.82	230.58	109.76
170	229.64	126.91	244.18	117.27
180	240.29	132.91	257.61	124.69
190	251.13	138.85	270.89	132.04
200	262.21	144.74	284.05	139.31
210	273.60	150.60	297.12	146.51
220	285.34	156.46	310.11	153.65
230	297.49	162.33	323.06	160.74
240	310.11	168.22	335.99	167.77
250	323.24	174.16	348.91	174.76
260	336.94	180.15	361.86	181.71
270	351.27	186.22	374.84	188.62
280	366.29	192.38	387.88	195.50

290	382.19	198.65	401.01	202.36
298.15	396.00	203.85	411.79	207.94
300	399.27	205.05	414.25	209.20
310	417.83	211.61	427.64	216.03
320	438.17	218.37	441.22	222.86
330	461.08	225.36	455.05	229.68
340	489.16	232.69	469.21	236.52
350	525.44	240.52	483.89	243.38
360	576.4	249.1	499.4	250.3
364.3	604.3	253.1	506.4	253.3
		Phase transition		
SmB_{Cr} phase				
364.3	544.32	319.8	573.0	253.3
370	558.61	323.3	581.6	258.2
371.8	563.1	324.5	584.3	259.8
		Phase transition		
SmA_d phase				
371.8	664	334	594	259.8
375.2	663	337	600	263
		Phase transition		
Isotropic liquid				
375.2	589.8	354	617	263
380	588.16	357	624	267

Table S4. Standard thermodynamic quantities of 5ABCA.

T / K	C_p / J K^{-1} mol^{-1}	$[H°(T) - H°(0)] / T$ / J K^{-1} mol^{-1}	$S°(T) - S°(0)$ / J K^{-1} mol^{-1}	$-[G°(T) - H°(0)] / T$ / J K^{-1} mol^{-1}
Crystal (K_{III})				
10	7.70	2.44	3.39	0.955
20	26.51	9.48	14.09	4.62
30	48.74	18.86	29.05	10.19
40	69.05	28.92	45.91	16.99
50	87.06	38.79	63.30	24.51
60	103.14	48.20	80.62	32.42
70	117.66	57.10	97.63	40.53
80	131.01	65.51	114.22	48.70
90	143.54	73.49	130.38	56.89
100	155.58	81.10	146.13	65.03
110	167.26	88.41	161.51	73.10
111.5	168.98	89.48	163.78	74.31
		Phase transition		
Crystal (K_{II})				
111.5	168.98	98.18	172.48	74.31
120	178.63	103.54	185.25	81.71
130	189.77	109.74	199.99	90.25
140	200.72	115.85	214.46	98.60
150	211.57	121.87	228.67	106.80
160	222.36	127.81	242.67	114.86
170	233.17	133.69	256.48	122.78
180	244.07	139.52	270.11	130.59
190	255.10	145.31	283.60	138.29
200	266.34	151.08	296.97	145.89
210	277.86	156.85	310.25	153.40
220	289.71	162.61	323.44	160.83
230	301.96	168.41	336.59	168.19
240	314.68	174.23	349.71	175.48

250	327.87	180.11	362.82	182.71
260	341.18	186.05	375.94	189.89
270	354.39	192.04	389.06	197.02
280	367.65	198.08	402.19	204.11
290	381.14	204.16	415.33	211.17
298.15	392.43	209.15	426.05	216.90
300	395.03	210.29	428.48	218.20
310	409.50	216.48	441.67	225.19
320	424.74	222.75	454.91	232.16
330	440.69	229.11	468.22	239.11
332	444.0	230.4	470.9	240.5
		Phase transition		
SmB_{Cr} phase				
332	510.13	289.6	530.1	240.5
340	520.61	294.9	542.4	247.5
350	535.99	301.6	557.7	256.1
360	556.0	308.4	573.1	264.7
363.3	563.2	310.7	578.2	267.5
		Phase transition		
SmA_d phase				
363.3	668	322	590	267.5
365.6	667	324	594	270
		Phase transition		
Isotropic liquid				
365.6	580.7	339	609	270
370	580.86	342	616	274
380	581.15	349	631	283

Table S5. Functions of layer spacing (c, d) against n in SmB_{Cr} and SmA_d phases in nABCA, nCBAA, and nBBAA.

Mesogen	Phase	Layer spacing against n
nABCA	SmB_{Cr}	c / Å = 1.4 × n + 13.3
	SmA_d	d / Å = 1.4 × n + 13.0
nCBAA	SmB_{Cr}	c / Å = 1.4 × n + 13.5
	SmA_d	d / Å = 1.4 × n + 13.2
nBBAA	SmB_{Cr}	c / Å = 1.4 × n + 14.4
	SmA_d	d / Å = 1.4 × n + 13.9

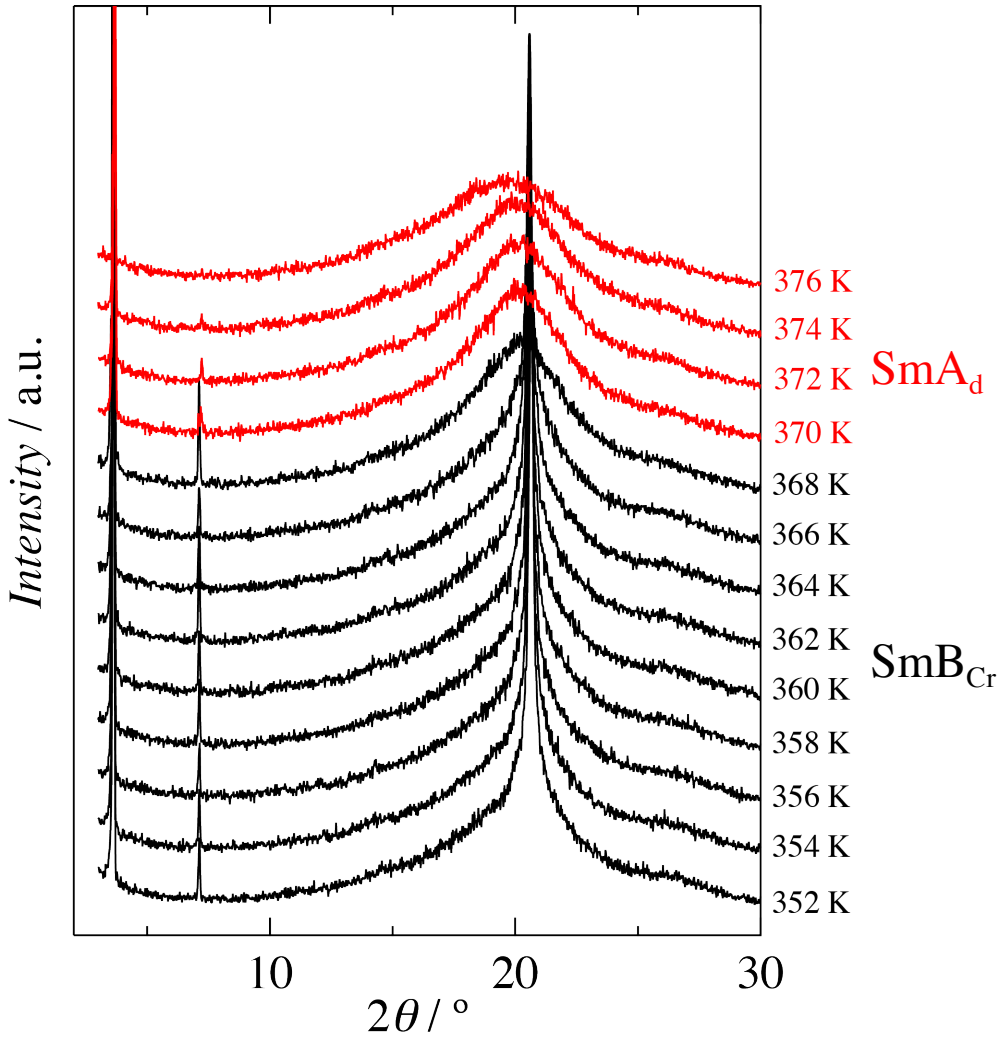

Fig. S1. X-ray diffraction patterns of SmA_d and SmB_{Cr} phases of 8CBAA at various temperatures (not corrected).