Supplementary material (ESI) for Journal of Materials Chemistry

Electronic Supplementary Information

New bent-core mesogens with carbon-carbon multiple linkages in the terminal chains

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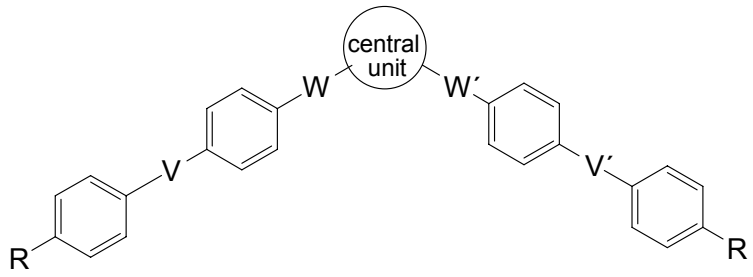
Analytical data:

Analytical data are given for the compounds **A16/in-11** and **B14/in-3** as representatives for members of series **A** and **B**:

Bis[4-(4-n-hexadec-11-inyloxycarbonylbenzylideneamino)phenyl] isophthalate **(A16/in-11)**
Melting behaviour: see Table 1
Elemental analysis: $C_{68}H_{80}O_8N_2$ (Mm = 1053.34); C 77.53, H 7.66, N 2.66 (calc.); C 77.18, H 7.83, N 2.31 (found);
^{1}H-NMR (400 MHz, $CDCl_3$): δ 0.88 (m, 6H, CH_3), 1.29-1.52 (m, 36H, CH_2), 1.78 (m, 4H, ArCOOCH$_2$*CH$_2$*), 2.12 (m, 8H, *CH$_2$*C≡C*CH$_2$*), 4.33 (t, ^3J = 6.7 Hz, 4H, ArCOO*CH$_2$*CH$_2$), 7.30 (m, 8H, Ar-H), 7.69 (t, ^3J = 7.9 Hz, 1H, Ar-H), 7.97 (d, ^3J = 8.5 Hz, 4H, Ar-H), 8.13 (d, ^3J = 8.5 Hz, 4H, Ar-H), 8.47 (m, 2H, Ar-H), 8.53 (s, 2H, CH=N), 9.03 (s, 1H, Ar-H).

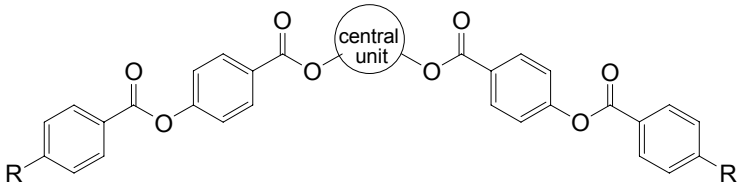
Bis{4-[2-(4-n-tetradec-3-inyloxycarbonyl)ethenylbenzylideneamino]phenyl} isophthalate **(B14/in-3)**
Melting behaviour: see Table 2
Elemental analysis: $C_{68}H_{76}O_8N_2$ (Mm = 1049.31): C 77.83, H 7.30, N 2.67 (calc.);C 77.54, H 7.45, N 2.40 (found);
^{1}H-NMR (400 MHz, $CDCl_3$): δ 0.86 (t, ^{3}J = 6.9 Hz, 6H, CH_3), 1.23-1.51 (m, 32H, CH_2), 2.14 (m, 4H, ArCH=CHCOOCH$_2$CH$_2$C≡C*CH$_2$*CH$_2$), 2.56 (m, 4H, ArCH=CHCOOCH$_2$*CH$_2$*C≡CCH$_2$), 4.28 (t, ^3J = 6.9 Hz, 4H, ArCOO*CH$_2$*CH$_2$C≡CCH$_2$), 6.52 (d, ^3J = 16.0 Hz, 2H, ArCH=*CH*COOCH$_2$), 7.29 (m, 8H, ArH), 7.62 (d, ^3J = 8.5 Hz, 4H, Ar-H), 7.69 (t, ^3J = 7.5 Hz, 1H, Ar-H), 7.72 (d, ^3J = 16.0 Hz, 2H, Ar*CH*=CHCOOCH$_2$), 7.92 (d, ^3J = 8.3 Hz, 4H, Ar-H), 8.47 (m, 2H, Ar-H), 8.48 (s, 2H, CH=N), 9.02 (s, 1H, Ar-H).

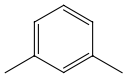
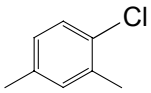
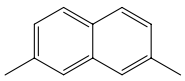
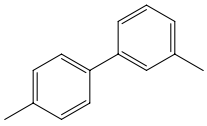
Table S1: References of bent-core mesogens containing different unsaturated chains R at one or both terminal positions (R is related to the general formula shown in Scheme 1)



-R	**n**	**R** at one terminal position	**R** at both terminal positions
-O-$(CH_2)_n$-CH=CH_2	9, 8	[S1-S7]	[S6, S10-S14]
-COO-$(CH_2)_n$-CH=CH_2	8		[S12]
-O-$(CH_2)_{10}$CH=CHCH_3 *(cis)*			[S15]
-O-$(CH_2)_8$CH=CHC_8H_{17} *(cis)*			[S15]
-O-$(CH_2)_n$OOCCH=CH_2	11,12	[S8]	[S15-S17]
-O-$(CH_2)_n$OOCC(CH_3)=CH_2	6,11,12	[S8]	[S15-S16]
-O-$(CH_2)_n$CH=CH-CH=CH_2	8, 10, 14		[S18]
-O-$(CH_2)_6OCH_2$CH=CH_2		[S9]	

Table S 2: Effect of the insertion of C=C bonds into both terminal chains on the mesophase behaviour of bent-core mesogens with increasing aromatic core. ΔT means the depression of the clearing temperatures caused by replacement the undecyloxy with undecenyloxy chains.



Central unit	R-	Mesophase behaviour	ΔT
	$C_{11}H_{23}O$-	Cr 105 $SmCP_A$ 113 I [S10]	
	CH_2=CH-$C_9H_{18}O$-	Cr 101 $SmCP_A$ 95 I [S11]	ΔT = -18K
	$C_{11}H_{23}O$-	Cr 85 N 113 I [S19]	
	CH_2=CH-$C_9H_{18}O$-	Cr 79 N 83 I [S11]	ΔT = -20K
	$C_{11}H_{23}O$-	Cr 136 $SmCP_A$ 169 I [S20]	
	CH_2=CH-$C_9H_{18}O$-	Cr 126 $SmCP_A$ 158 I [S12]	ΔT = -11K
	$C_{11}H_{23}O$-	Cr 87 Col_r 157 I [S21]	
	CH_2=CH-$C_9H_{18}O$-	Cr 99 Col_r 146 I [S10]	ΔT = -11K

Figs. S1 – S6: POM images of compound **A14/in-3** for further studies of the growing process of spiral filaments of different shape, myelinic-like and banana leaf-like domains, ribbon-like or circular domains, which can simultaneously occur in the same sample (thickness 6 µm and 10 µm) on slow cooling the isotropic liquid.

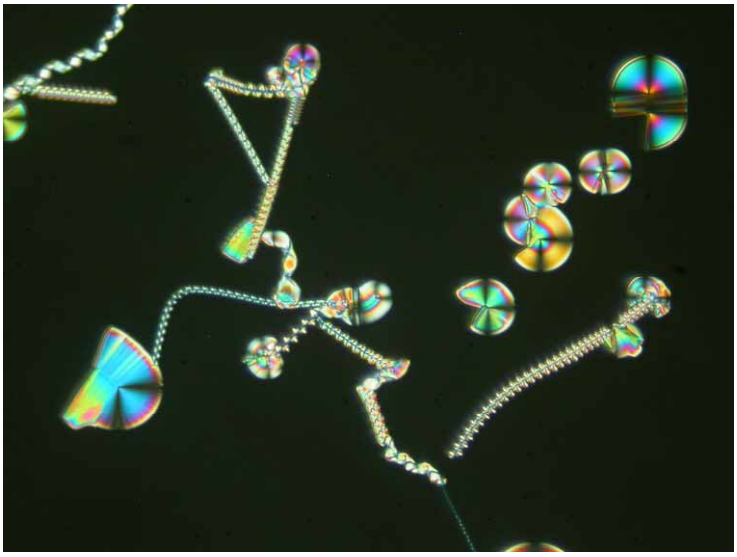


Fig. S1

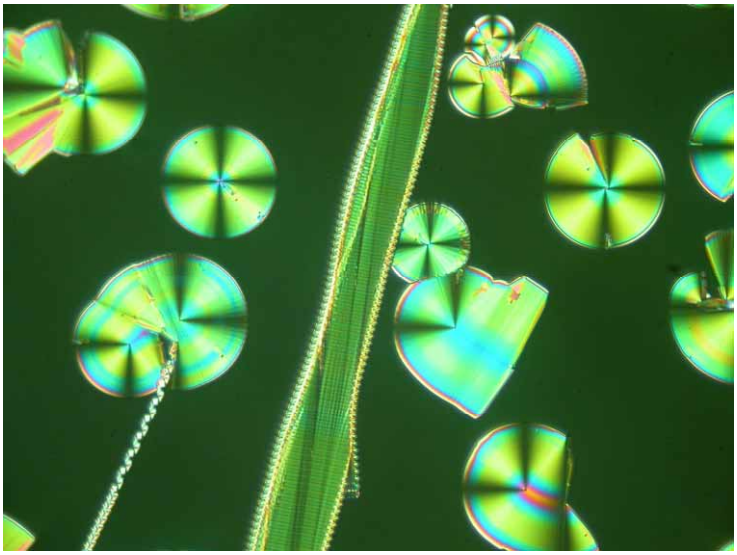


Fig. S2

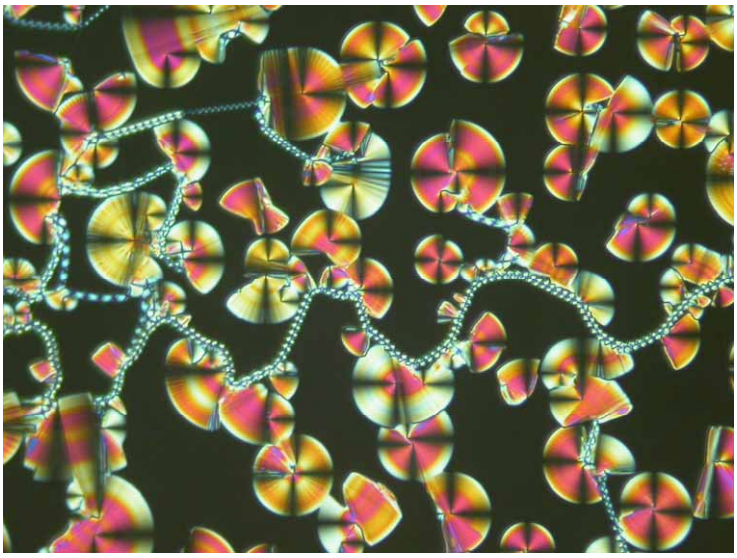


Fig. S3

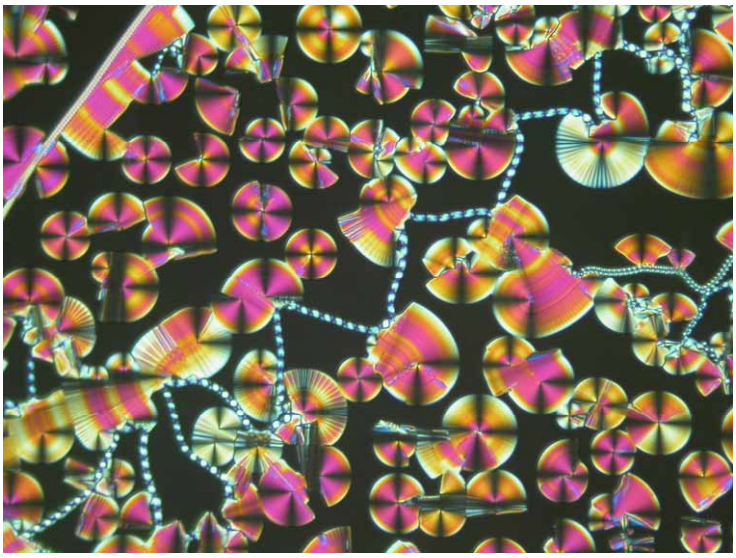


Fig. S4

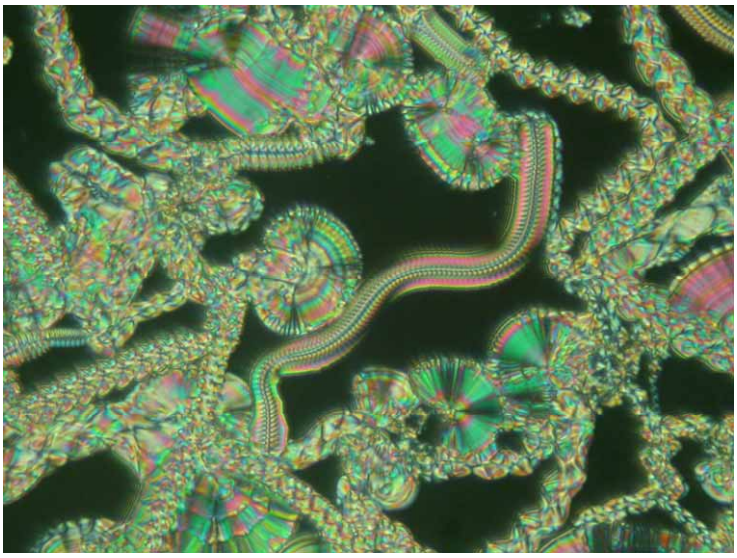


Fig. S5

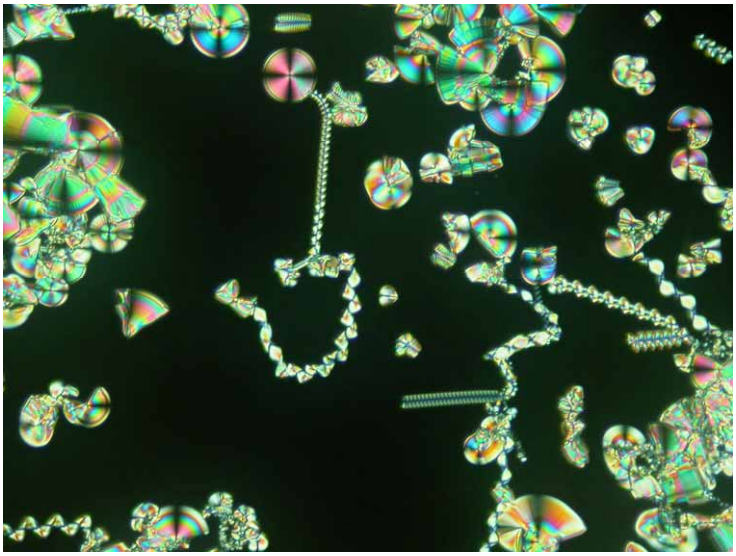


Fig. S6

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