Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Liquid crystalline and charge transport properties of novel non-peripherally octasubstituted perfluoroalkylated phthalocyanines

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ELECTRONIC SUPPORTING INFORMATION

Table S1. XRD lattice parameters of compounds **2** (a) and **3** (b) at both Col_h and Col_r mesophases

Fig. S1. Normalised UV-Visible spectra for compounds **1**,**2** and **3** in THF ($C=1x10^{-5}M$).

Fig. S2. DSC curves of **3** at 1°C / min of heating and cooling rates.

Fig. S3. Detailed POM analysis of mesophase textures of **2** upon cooling (1°C/min) from the isotropic phase in which we can observe the homeotropic alignment at the Col_h phase (a) followed by the Colr phase (b) with a *c2mm* symmetry which then rearranges into *p2gg* (c) until reaching its crystalline phase (d).

Fig. S4. XRD evidence for the symmetry rearrangement (*c2mm* to *p2gg*) occurring in the fluorinated phthalocyanine **2** as the columnar hexagonal phase collapses into Colr upon cooling (170 to 160°C).

Fig. S5. Nodal patterns of the a, s, -a and –s molecular orbitals (HOMO/LUMO) of the non-fluorinated phthalocyanine in B3LYP geometry optimisations with 6-31G(d) basis sets at an isosurface value of 0.03 au.

Table S1. XRD lattice parameters of mesophases for (a) **2** and (b) **3**

a)

T = 190 °C	**Col_h, a = 22.3 Å**	
hk	d_{obs}/ Å	$d_{theoretical}$/ Å
10	19.32	19.32
11	11.16	11.15
20	9.77	9.66
	5.5br	
	4.5br	
Z	1.0	1

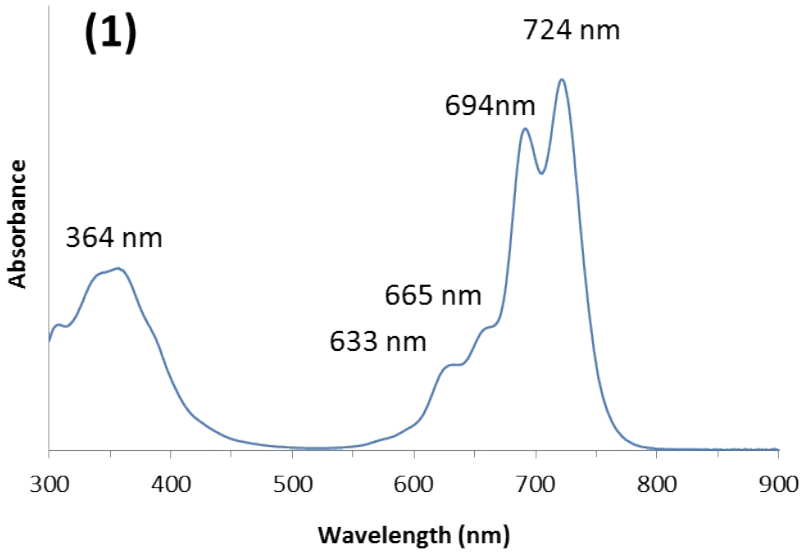
T = 170 °C	***Col_r (c2mm), a = 41.7 Å***
hk	d_{obs}/ Å
11	19.62
20	20.82
13	7.28
22	9.76
40	10.38
	5.4br
	4.4sh, br
Z	1.9

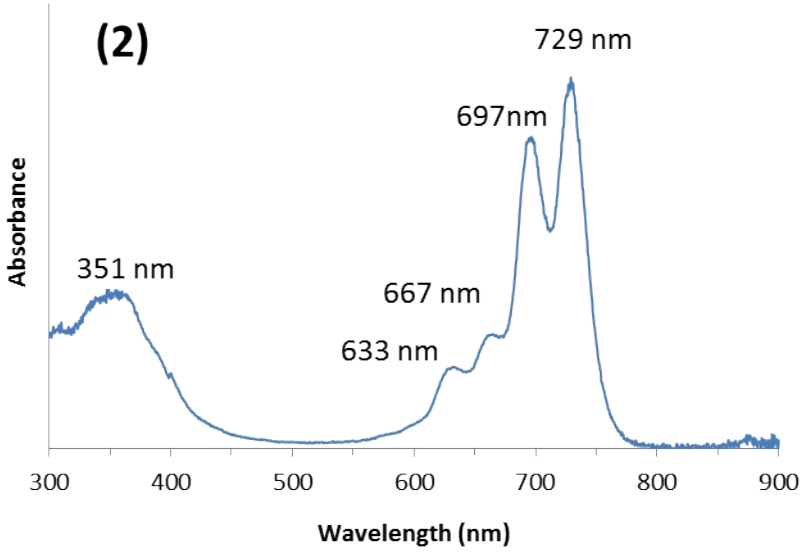
T = 160 °C	**Col_r (*p2gg*), a = 41.7 Å, b = 22.4 Å**	
hk	d_{obs}/ Å	$d_{theoretical}$/ Å
11	19.70	19.70
20	20.87	20.87
13	7.28	7.34
22	9.82	9.85
40	10.35	10.44
32	8.84	8.71
52	6.84	6.69
	5.4br	
	4.4sh, br	
Z	1.9	2

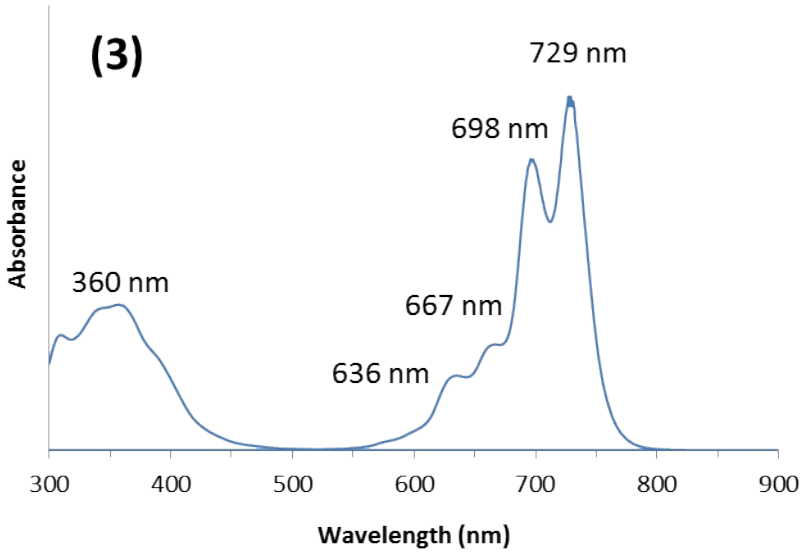
b)

T = 155 °C	**Col_h, a = 21.7 Å**	
hk	d_{obs}/ Å	$d_{theoretical}$/ Å
10	18.79	18.79
11	10.85	10.85
20	9.41	9.40
	4.5br	
Z	1.1	1

T = 140 °C	**Col_r (*c2mm*), a = 38.5 Å, b = 21.3 Å**	
hk	d_{obs}/ Å	$d_{theoretical}$/ Å
11	18.63	18.63
20	19.24	19.24
2	10.63	10.65
22	9.31	9.31
40	9.59	9.62
	4.4br	
Z	2.0	2







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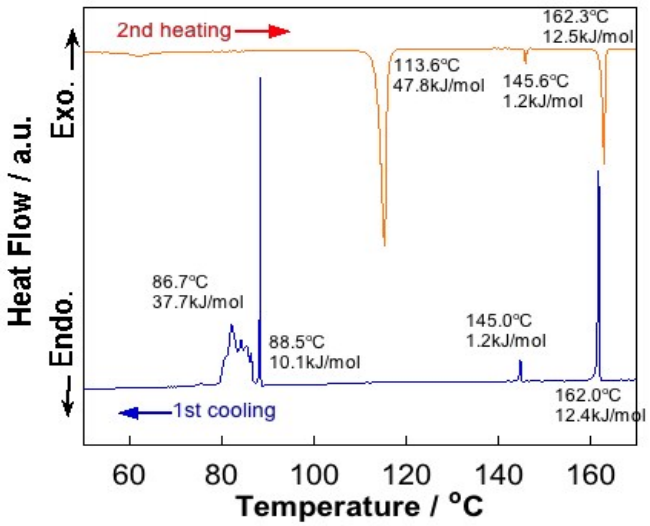
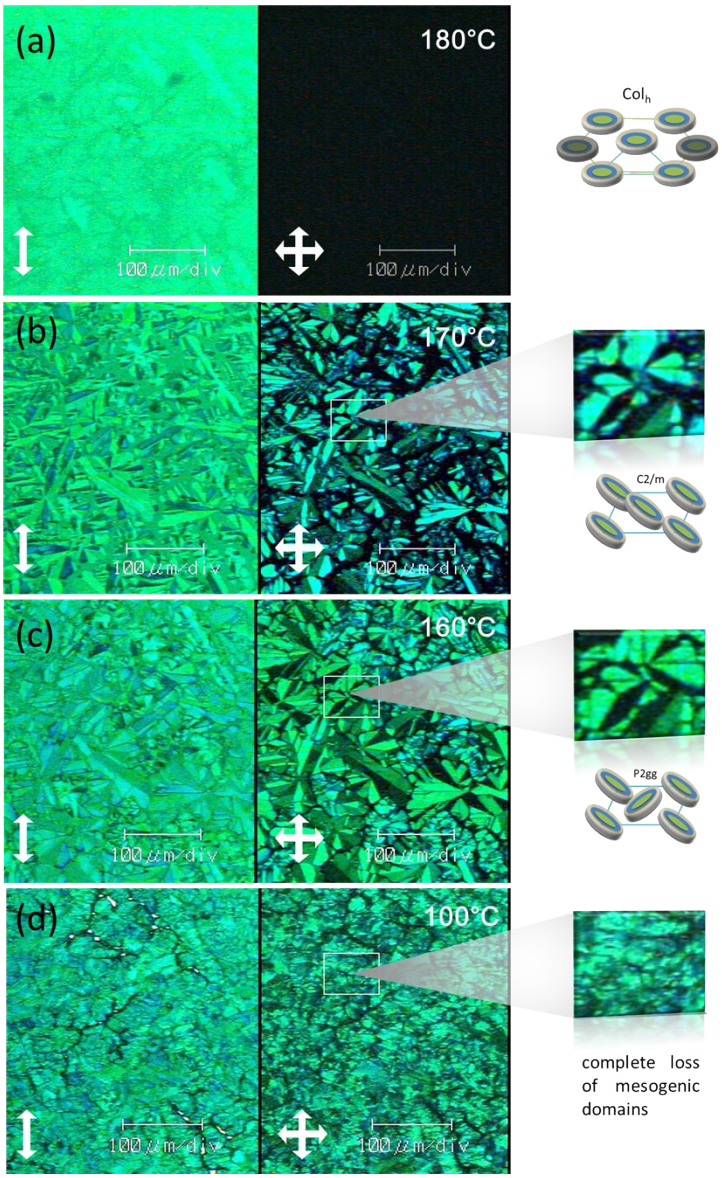


Fig. S2. DSC curves of **3** at 1°C / min of heating and cooling rates.



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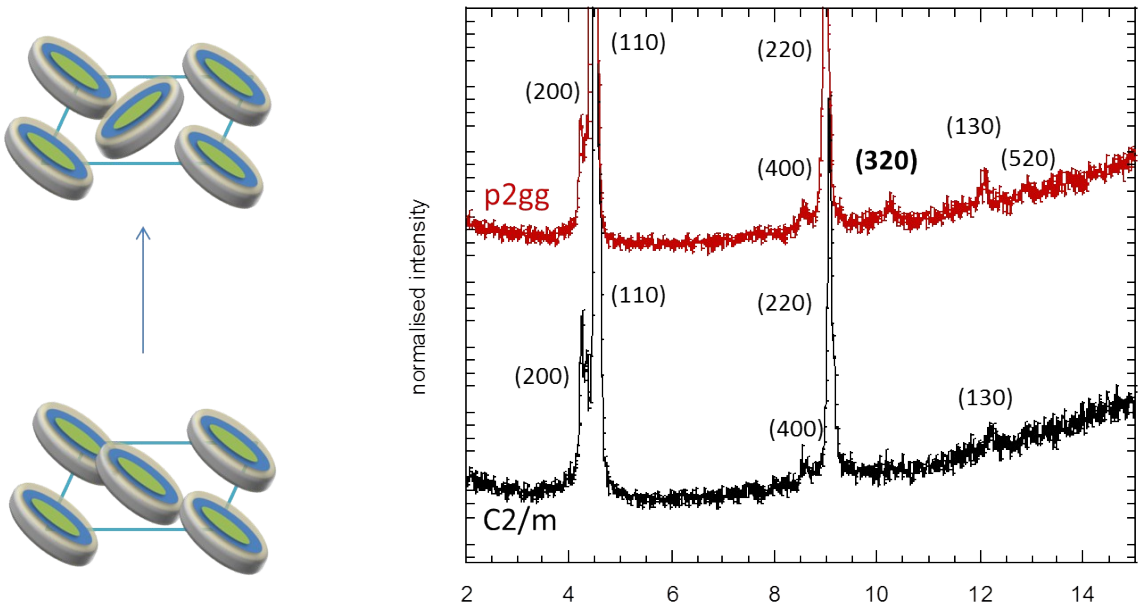

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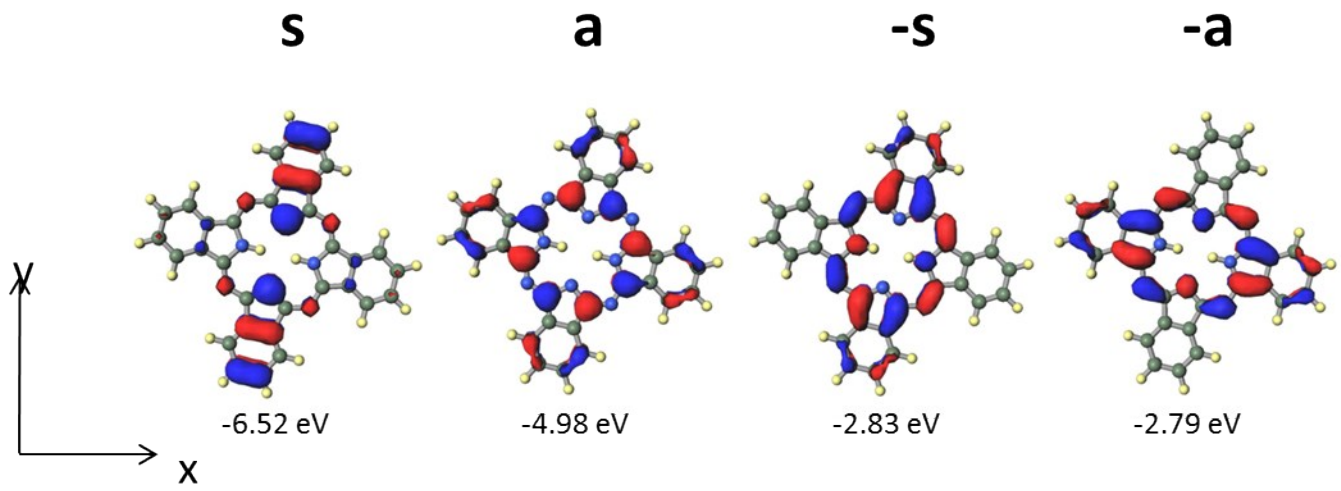

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