Supporting Information for

The effect of terminal substituents on crystal structure, mesophase behaviour and optical property of azo-ester linked materials

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Table SI1: FT-IR vibrational frequencies for main functional groups and ¹H NMR chemical shifts of different type of protons present in compounds **C1-C6**

Wavenumber (cm ⁻¹)					
Functional groups	(C–H, aliphatic)	(C=O in ester)	(C=C, vinyl)	(C=C, aromatic)	(–N=N–)
C1	2945, 2880	1725	1634	1603, 1583	1505, 1471
C2	2945, 2874	1729	1638	1606, 1573	1506, 1489
C3	2944, 2871	1736	1637	1602, 1583	1503, 1486
C4	2956, 2881	1717	1632	1605, 1584	1507, 1473
C5	2957, 2873	1722	1642	1605, 1584	1505, 1473
C6	2946, 2872	1724	1637	1604, 1596	1508, 1476

Chemical Shift (ppm)								
Type of protons	Ar– <u>H</u>	–CH=CH ₂	–CH=CH ₂	–CH=CH ₂	Ar–OCH ₂ –	–CH ₂ –OCO–	–OCH ₃	–CH ₂ –
C1	8.33-6.98	6.43-6.37	6.16-6.06	5.84-5.79	4.21-4.15	4.09-4.02	-	1.89-1.41
C2	8.33-6.98	6.43-6.37	6.16-6.08	5.85-5.79	4.21-4.15	4.09-4.02	-	1.89-1.41
C3	8.34-6.98	6.43-6.37	6.16-6.08	5.84-5.79	4.22-4.15	4.09-4.02	-	1.90-1.42
C4	8.32-6.90	6.42-6.35	6.15-6.06	5.83-5.77	4.19-4.14	4.07-4.01	3.82-3.78	1.88-1.42
C5	8.35-6.90	6.42-6.40	6.15-6.07	5.84-5.78	4.22-4.14	4.09-4.00	-	1.89-1.39
C6	8.32-6.90	6.42-6.40	6.16-6.07	5.88-5.78	4.20-4.14	3.95-3.89	-	1.88-1.00

Table SI2: Selected bond lengths (Å) and bond angles (°) of compounds **C1**, **C4** and **C5**

Bond lengths (Å)	C1	C4	C5	Bond angles (°)	C1	C4	C5
F(1)-C(26)	1.361(3)	-	-	F(1)-C(26)-C(25)	118.6(2)	-	-
N(1)-N(2)	1.256(2)	1.2603(18)	1.2506(19)	N(2)-N(1)-C(13)	113.52(18)	114.23(13)	112.81(15)
N(1)-C(13)	1.419(3)	1.4149(19)	1.420(2)	N(1)-N(2)-C(16)	114.84(18)	113.33(13)	116.16(15)
N(2)-C(16)	1.423(3)	1.4278(19)	1.418(2)	C(3)-O(2)-C(4)	115.19(18)	117.35(12)	116.81(14)
O(1)-C(3)	1.205(3)	1.2075(18)	1.198(2)	C(10)-O(3)-C(9)	117.94(17)	118.32(12)	120.24(14)
O(2)-C(3)	1.344(3)	1.3399(18)	1.330(2)	C(22)-O(5)-C(23)	119.19(16)	120.98(12)	122.57(15)
O(3)-C(10)	1.361(3)	1.3587(18)	1.359(2)	C(1)-C(2)-C(3)	121.5(2)	120.93(15)	122.8(2)
O(4)-C(22)	1.205(2)	1.2015(19)	1.194(2)	H(1A)-C(1)-H(1B)	120.0	120.0	120.0
O(5)-C(22)	1.363(2)	1.3543(19)	1.352(2)	O(1)-C(3)-O(2)	123.6(2)	123.43(14)	124.53(19)
O(6)-C(29)	-	1.428(2)	1.427(2)	O(2)-C(4)-H(4B)	109.9	110.5	110.1
C(1)-H(1A)	0.9300	0.9300	0.9300	C(4)-C(5)-C(6)	111.0(2)	113.32(13)	112.35(16)
C(1)-H(1B)	0.9300	0.9300	0.9300	O(3)-C(9)-C(8)	108.10(18)	107.44(12)	107.05(15)
C(2)-C(3)	1.478(3)	1.480(2)	1.459(3)	C(13)-C(12)-C(11)	120.9(2)	119.3	120.57(17)
C(4)-H(4A)	0.9700	0.9700	0.9700	C(12)-C(13)-N(1)	116.75(19)	116.29(14)	123.61(16)
C(5)-(6)	1.520(3)	1.520(2)	1.510(2)	C(17)-C(16)-N(2)	124.94(19)	124.24(14)	114.55(16)
C(11)-H(11)	0.9300	0.9300	0.9300	C(21)-C(16)-N(2)	115.19(19)	115.86(13)	126.14(16)
C(14)-C(15)	1.371(3)	1.371(3)	1.385(2)	C(21)-C(20)-C(19)	120.39(19)	119.81(14)	121.01(17)
C(18)-H(18)	0.9300	0.9300	0.9300	C(28)-C(23)-O(5)	121.8(2)	115.49(13)	125.33(18)
C(19)-C(22)	1.478(3)	1.485(2)	1.476(3)	C(23)-C(28)-C(27)	118.7(2)	120.12(14)	120.16(19)
C(23)-C(24)	1.378(3)	1.391(2)	1.372(3)	O(6)-C(26)-C(27)	-	125.02(15)	125.01(18)
C(26)-C(27)	1.374(3)	1.387(2)	1.372(3)	C(29)-C(30)-H(30B)	-	-	109.5
C(29)-C(30)	-	-	1.492(3)				

Table SI3: Thermal analysis data for compounds **C1- C6**

	T _d (5%) (°C)	1 st decomposition		2 nd decomposition		Char yield (%)
		Temp.(°C)	Wt. loss (%)	Temp.(°C)	Wt. loss (%)	
C1	316	271-392	36	392-556	35	23
C2	318	264-435	48	435-543	21	20
C3	317	284-389	51	403-474	13	16
C4	318	266-352	38	352-536	33	24
C5	317	265-391	40	391-535	32	18
C6	319	266-400	43	400-525	27	15

Figure SI1: Crystal structure of compound **C4** with the hydrogen bond motifs

Figure SI2: Crystal structure of compound **C5** with the hydrogen bond motifs