Supplemental information

The effect of orientation of the lateral methyl substituent on the mesophase behavior of 4-alkoxyphenylazo aryl benzoates

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Table S1. FT-IR absorption spectra of compounds **II**8_{a-f} and **III**12_{a-f}.

Compound	X	V _{CH3} Asym.	V _{CH3} Sym.	VC=O	VC=N	VC-O	VC-O	VNO ₂	VC≡N
II 8 _a	CH ₃ O	2927	2857	1730	1603	1469	1244	-	-
II 8 _b	CH ₃	2925	2855	1738	1605	1467	1246	-	-
II 8 _c	H	2925	2855	1740	1602	1465	1254	-	-
II 8 _d	Br	2926	2856	1740	1592	1469	1255	-	-
II 8 _e	NO ₂	2925	2855	1739	1602	1469	1254	1526 1349	-
II 8 _f	CN	2925	2855	1739	1602	1466	1252	-	2227
III 12 _a	CH ₃ O	2928	2856	1734	1603	1470	1253	-	-
III 12 _b	CH ₃	2921	2851	1737	1603	1471	1250	-	-
III 12 _c	H	2924	2853	1738	1601	1469	1254	-	-
III 12 _d	Br	2922	2853	1736	1590	1467	1256	-	-
III 12 _e	NO ₂	2929	2855	1735	1608	1476	1250	1524 1325	-
III 12 _f	CN	2923	2853	1739	1604	1475	1250	-	2230

Table S2. ¹H-NMR spectra (in ppm) of compounds **II**8_{a-f} and **III**/2_{a-f}.

Comp No.	X	Y	1 t,3H	2 m,18H	3 q,2H	4 t,2H	5 d,2H	6 d,2H	7 d,1H	8 d,2H	9 s,3H	10 d,2H	11 d,2H	12 s,3H (t,1H)*
II 8 _a	CH ₃ O	2-CH ₃	0.85	1.30	1.78	3.98	6.95	7.85	7.82	7.19	2.25	8.14	6.96	3.84
II 8 _b	CH ₃	2-CH ₃	0.93	1.37	1.84	4.06	7.00	7.92	7.81	7.27	2.34	8.14	7.03	2.48
II 8 _c	H	2-CH ₃	3-CH ₃	0.84	1.43	1.75	4.08	6.90	7.91	7.63	7.26	2.69	8.14	7.38
II 8 _d	Br	2-CH ₃	0.94	1.37	1.72	4.07	7.00	7.81	7.86	7.27	2.48	8.17	7.02	
II 8 _e	NO ₂	2-CH ₃	0.96	1.33	1.71	3.94	6.97	7.82	7.81	7.23	2.38	8.40	8.34	
II 8 _f	CN	2-CH ₃	0.96	1.33	1.71	3.94	6.97	7.82	7.81	7.23	2.36	8.32	7.66	
III /2 _a	CH ₃ O	3-CH ₃	0.86	1.31	1.73	4.01	6.94	7.89	7.80	7.21	2.23	8.15	7.01	3.85
III /2 _b	CH ₃	3-CH ₃	0.85	1.43	1.75	4.08	7.11	7.90	7.63	7.21	2.68	8.05	7.36	2.43
III /2 _c	H	3-CH ₃	0.84	1.43	1.75	4.08	6.90	7.91	7.63	7.26	2.69	8.14	7.38	(7.65)*
III /2 _d	Br	3-CH ₃	0.85	1.43	1.74	4.08	7.11	7.90	7.63	7.37	2.68	8.06	7.38	-
III /2 _e	NO ₂	3-CH ₃	0.85	1.43	1.75	4.08	7.11	7.90	7.65	7.28	2.69	8.39	7.42	-
III /2 _f	CN	3-CH ₃	0.85	1.43	1.75	4.08	7.11	7.90	7.64	7.27	2.69	8.28	7.41	-

*Data for unsubstituted derivative

Table S3. Mass spectra of compounds **II**8_{a-f} and **III**/2_{a-f}.

Comp No.	<i>n</i>	X	Y	Molar mass	C _n H _{n+1} OC ₆ H ₄ N ₂ – C ₆ H ₃ (Y)O	OC ₆ H ₄ N ₂ – C ₆ H ₃ (Y)O	OC ₆ H ₄ N ₂	X-C ₆ H ₄ CO	.OC ₆ H ₄ N ₂ – C ₆ H ₃ (Y)OCOC ₆ H ₄ X
II 8 _a	8	CH ₃ O	2-CH ₃	474	339	227	120	135	361
II 10 _b	10	CH ₃	2-CH ₃	486	367	227	120	119	345
II 10 _c	10	H	2-CH ₃	472	367	227	120	105	331
II 8 _d	8	Br	2-CH ₃	524	339	227	120	183	411
II 8 _e	8	NO ₂	2-CH ₃	489	339	227	120	150	376
II 8 _f	8	CN	2-CH ₃	469	339	227	120	130	356
III /2 _a	12	CH ₃ O	3-CH ₃	530	395	227	120	135	361
III /2 _b	12	CH ₃	3-CH ₃	514	395	227	120	119	345
III /2 _c	12	H	3-CH ₃	500	395	227	120	105	331
III /2 _d	12	Br	3-CH ₃	580	395	227	120	183	411
III /2 _e	12	NO ₂	3-CH ₃	545	395	227	120	150	376
III /2 _f	12	CN	3-CH ₃	525	395	227	120	130	356

Table S4. Elemental analyses calculated (and found) for 4-(4'-alkoxy phenylazo) 2-methyl phenyl 4''-substituted benzoates, **II**_n-f.

Comp	<i>n</i>	X	Mol. wt	Elemental analysis Cal. (Found)			
				% C	% H	% N	% Br
II 6 _a		OCH ₃	446.55	77.62 (77.57)	6.77 (6.75)	6.27 (6.33)	-
II 6 _b		CH ₃	430.55	75.32 (75.30)	7.02 (7.04)	6.51 (6.53)	-
II 6 _c		H	416.52	74.97 (74.87)	6.78 (6.57)	6.73 (6.50)	-
II 6 _d		Br	495.42	63.03 (63.05)	5.49 (5.45)	5.65 (5.63)	16.13 (16.16)
II 6 _e		NO ₂	461.52	67.66 (67.33)	5.90 (5.92)	9.10 (9.80)	-
II 6 _f		CN	441.53	73.45 (73.42)	6.16 (6.13)	9.52 (9.53)	-
II 8 _a	8	OCH ₃	474.60	73.39 (73.61)	7.22 (7.45)	5.90 (6.02)	-
II 8 _b		CH ₃	458.60	75.95 (75.89)	7.47 (7.69)	6.11 (6.42)	-
II 8 _c		H	444.58	75.65 (75.93)	7.26 (7.59)	6.30 (6.56)	-
II 8 _d		Br	523.47	64.25 (64.45)	5.97 (6.14)	5.35 (5.49)	15.26 (15.39)
II 8 _e		NO ₂	489.57	68.69 (68.94)	6.38 (6.70)	8.58 (8.75)	-
II 8 _f		CN	469.59	74.18 (74.53)	6.65 (6.86)	8.95 (8.84)	-
II 10 _a	10	OCH ₃	502.66	74.07 (74.23)	7.62 (7.51)	5.57 (5.82)	-
II 10 _b		CH ₃	486.66	76.51 (76.76)	7.87 (7.70)	5.76 (5.48)	-
II 10 _c		H	472.63	76.24 (76.49)	7.68 (7.95)	5.93 (6.19)	-
II 10 _d		Br	551.53	65.33 (65.54)	6.40 (6.23)	5.08 (5.27)	14.49 (14.65)
II 10 _e		NO ₂	517.63	69.61 (69.87)	6.82 (6.66)	8.12 (8.39)	-
II 10 _f		CN	497.64	74.82 (74.97)	7.09 (7.36)	8.44 (8.71)	-
II 12 _a	12	OCH ₃	530.71	74.69 (74.41)	7.98 (7.69)	5.28 (5.49)	-
II 12 _b		CH ₃	524.71	77.01 (77.27)	8.22 (8.38)	5.44 (5.73)	-
II 12 _c		H	500.68	76.77 (76.95)	8.05 (8.30)	5.60 (5.86)	-
II 12 _d		Br	579.57	66.32 (66.63)	6.78 (6.96)	4.83 (4.98)	13.79 (13.91)
II 12 _e		NO ₂	545.68	70.44 (70.59)	7.20 (7.48)	7.70 (7.94)	-
II 12 _f		CN	525.69	75.40 (75.77)	7.48 (7.76)	7.99 (8.23)	-

Table S5. Elemental analyses calculated (and found) for 4-(4'-alkoxy phenylazo) 3-methyl phenyl 4''-substituted benzoates, **III***n*_{a-f}.

Comp.	<i>n</i>	X	Mol. wt	Elemental analysis Cal. (Found)			
				% C	% H	% N	% Br
III 6 _a	6	OCH ₃	446.55	77.62 (77.57)	6.77 (6.75)	6.27 (6.33)	-
III 6 _b		CH ₃	430.55	75.32 (75.30)	7.02 (7.04)	6.51 (6.53)	-
III 6 _c		H	416.52	74.97 (74.75)	6.78 (6.44)	6.73 (6.39)	-
III 6 _d		Br	495.42	63.03 (63.05)	5.49 (5.45)	5.65 (5.62)	16.13 (16.16)
III 6 _e		NO ₂	461.52	67.66 (67.63)	5.90 (5.92)	9.10 (9.80)	-
III 6 _f		CN	441.53	73.45 (73.42)	6.16 (6.13)	9.52 (9.53)	-
III 8 _a	8	OCH ₃	474.60	73.39 (73.55)	7.22 (7.58)	5.90 (6.07)	-
III 8 _b		CH ₃	458.60	75.95 (75.73)	7.47 (7.63)	6.11 (6.35)	-
III 8 _c		H	444.58	75.65 (75.87)	7.26 (7.55)	6.30 (6.48)	-
III 8 _d		Br	523.47	64.25 (64.59)	5.97 (6.04)	5.35 (5.51)	15.26 (15.47)
III 8 _e		NO ₂	489.57	68.69 (68.89)	6.38 (6.62)	8.58 (8.81)	-
III 8 _f		CN	469.59	74.18 (74.40)	6.65 (6.72)	8.95 (8.79)	-
III 10 _a	10	OCH ₃	502.66	74.07 (74.45)	7.62 (7.34)	5.57 (5.70)	-
III 10 _b		CH ₃	486.66	76.51 (76.69)	7.87 (7.64)	5.76 (5.33)	-
III 10 _c		H	472.63	76.24 (76.53)	7.68 (7.91)	5.93 (6.01)	-
III 10 _d		Br	551.53	65.33 (65.25)	6.40 (6.28)	5.08 (5.30)	14.49 (14.58)
III 10 _e		NO ₂	517.63	69.61 (69.93)	6.82 (6.57)	8.12 (8.33)	-
III 10 _f		CN	497.64	74.82 (74.95)	7.09 (7.26)	8.44 (8.62)	-
III 12 _a	12	OCH ₃	530.71	74.69 (74.44)	7.98 (7.76)	5.28 (5.45)	-
III 12 _b		CH ₃	524.71	77.01 (77.36)	8.22 (8.08)	5.44 (5.61)	-
III 12 _c		H	500.68	76.77 (76.83)	8.05 (8.24)	5.60 (5.77)	-
III 12 _d		Br	579.57	66.32 (66.54)	6.78 (6.92)	4.83 (5.01)	13.79 (13.98)
III 12 _e		NO ₂	545.68	70.44 (70.48)	7.20 (7.52)	7.70 (7.89)	-
III 12 _f		CN	525.69	75.40 (75.53)	7.48 (7.61)	7.99 (8.19)	-