Fluorinated liquid crystals formed by halogen bonding

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Electronic Supplementary Information

Experimental Methods

General. IR spectra were recorded with a Nicolet Nexus FT-IR spectrophotometer. Melting points were established with a Reichert instrument. DSC analysis was performed on a Linkam DSC 600 instrument with a heating rate of 10°C/min. Commercially available chemicals were used without further purification. ¹H and ¹⁹F NMR spectra were recorded on a Bruker ADV 500 spectrometer at 25 °C, CDCl₃ was used as solvent, TMS and CFCl₃ were used as internal standards. NMR spectra were registered in the presence of 2,2,2-trifluoroethyl ether as an internal standard. On calibrating integration parameters so that in ¹H NMR spectra the CH₂O quartet of 2,2,2-trifluoroethyl ether was corresponding to four and in ¹⁹F NMR spectra the CF₃ triplet of 2,2,2-trifluoroethyl ether was corresponding to six, the ratio of the –CF₂-I signal area (deriving from **2**) and the –CH₃ signal area (deriving from **1**) is 1:3 thus revealing that the **1:2** ratio in **3** is 2:1. Chemicals were purchased from *Sigma-Aldrich* and *Apollo Scientific*.

X-ray diffraction analysis. Single crystal X-ray structures were determined at room temperature by using a Bruker SMART-APEX diffractometer equipped with CCDC area detector.

General procedure for the synthesis of complexes 1. Good quality crystals of **1** were obtained by dissolving, in a vial of clear borosilicate glass at room temperature, the stilbazole and the diiodoperfluoroalkane in a 2:1 ratio. THF was used as solvent. The closed vial was stored at +6 °C and after a period ranging from one to five days yellow and transparent crystals were isolated.

1a: Mp (THF) 103 °C; FT IR (KBr/♥/ cm⁻¹, selected bands): 3071(vw), 3042(vw), 2957 (w), 2941(m), 2856(w), 1588-1573(s), 1511(s), 1259(s), 1185(s), 1117(s) 996(m), 824(s).

1b: Mp (THF) 99 °C; FT IR (KBr/♥/ cm⁻¹, selected bands): 3073 (vw), 3040(vw), 2930(w), 2856(w), 1591-1574(s), 1511(m), 1245(m), 1187(s), 1115(s), 996(m), 826(s).

1c: Mp (THF) 95 °C; FT IR (KBr/♥/ cm⁻¹, selected bands): 3072 (vw), 3028(vw), 2919(w), 2849(w), 1589(s), 1511(m), 1245(m), 1186(s), 1124(s), 996(m), 827(s).

1d: Mp (THF) 108 °C; FT IR (KBr/♥/ cm⁻¹, selected bands): 3070 (vw), 3036(vw), 2925(w), 2854(w), 1589-1572(s), 1511(m), 1249(m), 1205(s), 1137(s), 998(m), 825(s).

1e: Mp (THF) 110 °C; FT IR (KBr/√/ cm⁻¹, selected bands): 3072 (vw), 3027(vw), 2922(m), 2851(w), 1592-1573(s), 1511(m), 1247(m), 1213(s), 1134(s), 997(m), 827(s).

1f: Mp (THF) 100 °C; **FT IR (KBr/v/ cm⁻¹, selected bands**): 3070 (vw), 3025(vw), 2919(w), 2848(w), 1590(s), 1511(m), 1251(m), 1209(s), 140(s), 997(m), 831(s).