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. \(^1\)H and \(^{19}\)F NMR spectra were recorded on a Bruker ADV 500 spectrometer at 25°C, CDCl\(_3\) was used as solvent, TMS and CFCl\(_3\) 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 \(^1\)H NMR spectra the CH\(_2\)O quartet of 2,2,2-trifluoroethyl ether was corresponding to four and in \(^{19}\)F NMR spectra the CF\(_3\) triplet of 2,2,2-trifluoroethyl ether was corresponding to six, the ratio of the –CF\(_2\)-I signal area (deriving from 2) and the –CH\(_3\) 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/ν 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/ν 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/ν 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/ν 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/ν 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/ν 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).