Electronic Supplementary Material (ESI) for CrystEngComm.

Hydrogen-bonded Liquid Crystals formed from 4-Alkoxystilbazoles and Chlorophenols

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Supplementary Information

Preparation

Chlorophenols were obtained commercially, while stilbazoles were prepared using the Siegrist protocol described previously.[1][Huck]

Complexes were prepared dissolving the stilbazole (30 mmol) in pentane for **St8** or hexane for **St12** (50 cm^3 in each case) to which was added a solution of the chlorophenol (30 mmol) in the same solvent (10 cm^3). The solution was stirred for 90 minutes after which the flask was sealed with a suba seal through which was inserted a syringe needle. The flasks were then left at ambient temperature for 1-2 weeks until an appreciable yield of crystals was obtained. The crystals were recovered by filtration and washed carefully with cold solvent of crystallisation before being air-dried.

Single-crystal X-ray

Diffraction data were collected at 110 K on a Bruker Smart Apex diffractometer with Mo-K_α radiation (λ = 0.71073 Å) using a SMART CCD camera. Diffractometer control, data collection and initial unit cell determination was performed using 'SMART'.[2] The crystal was cooled with an Oxford Crysostream. Frame integration and unit-cell refinement was carried out with 'SAINT+'.[3] Absorption corrections were applied by SADABS.[4] Structures were solved by 'direct methods' using SHELXS-97 (Sheldrick, 1997)[5] and refined by full-matrix least squares using SHELXL-97 (Sheldrick, 1997).[6] All non-hydrogen atoms were refined anisotropically. O-H hydrogens were located by difference map after all other atoms had been located and refined.

Mesophase Characterisation

Polarised optical microscopy employed an Olympus BX50 Optical Microscope equipped with a Link-Am HFS91 hot stage, TMS92 controller and LNP2 cooling unit.

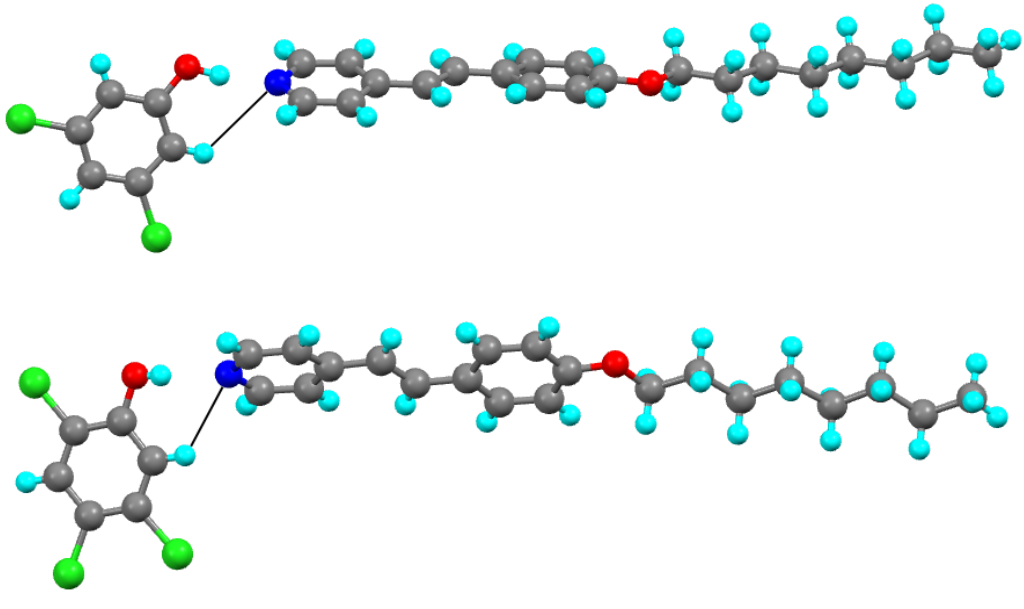

Figure S1 Hydrogen bonded complex for (a) **8St-b** and (b) **8St-d** showing possible intra-complex N···H interaction.

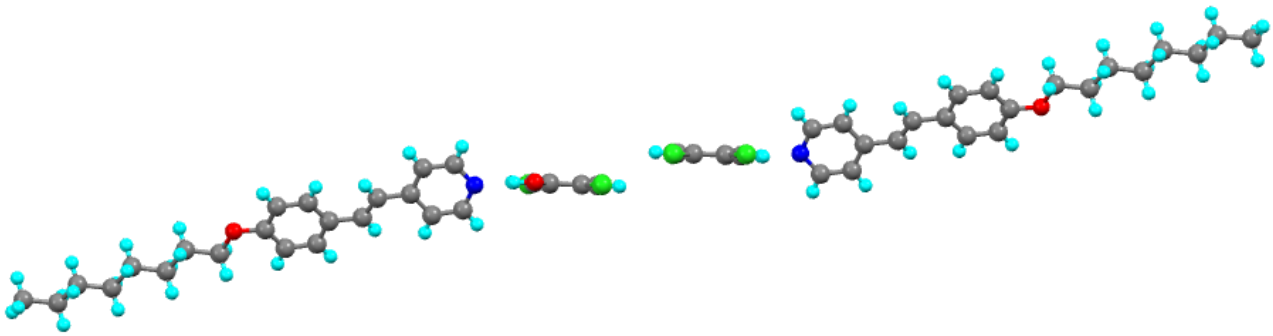

Figure S2 Side view of the dimeric unit in the structure of **8St-e**.

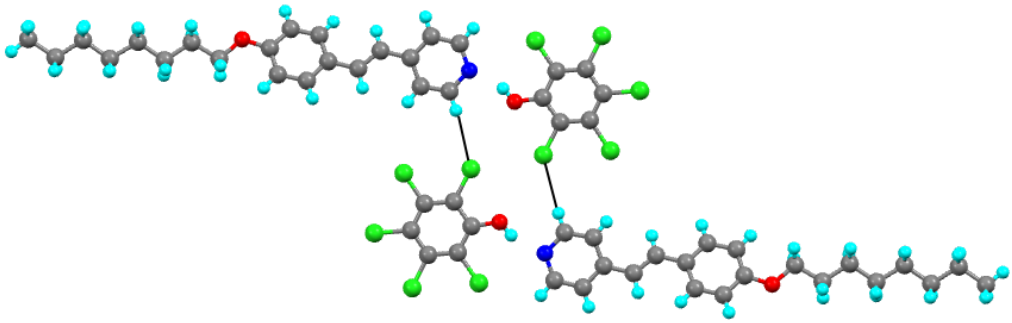

Figure S3 Diagram to show the possible inter-complex Cl···H interactions in **8St-f**.

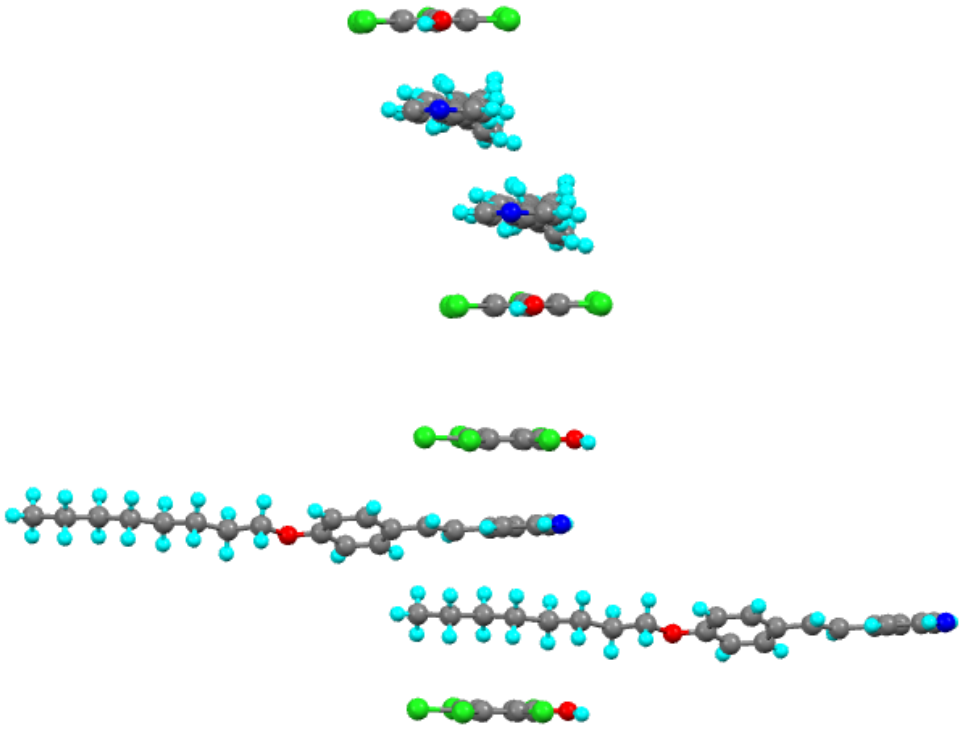

Figure S4 Two different side-on views (effectively perpendicular to the *b*-axis) of the stacking in **St8-f**.

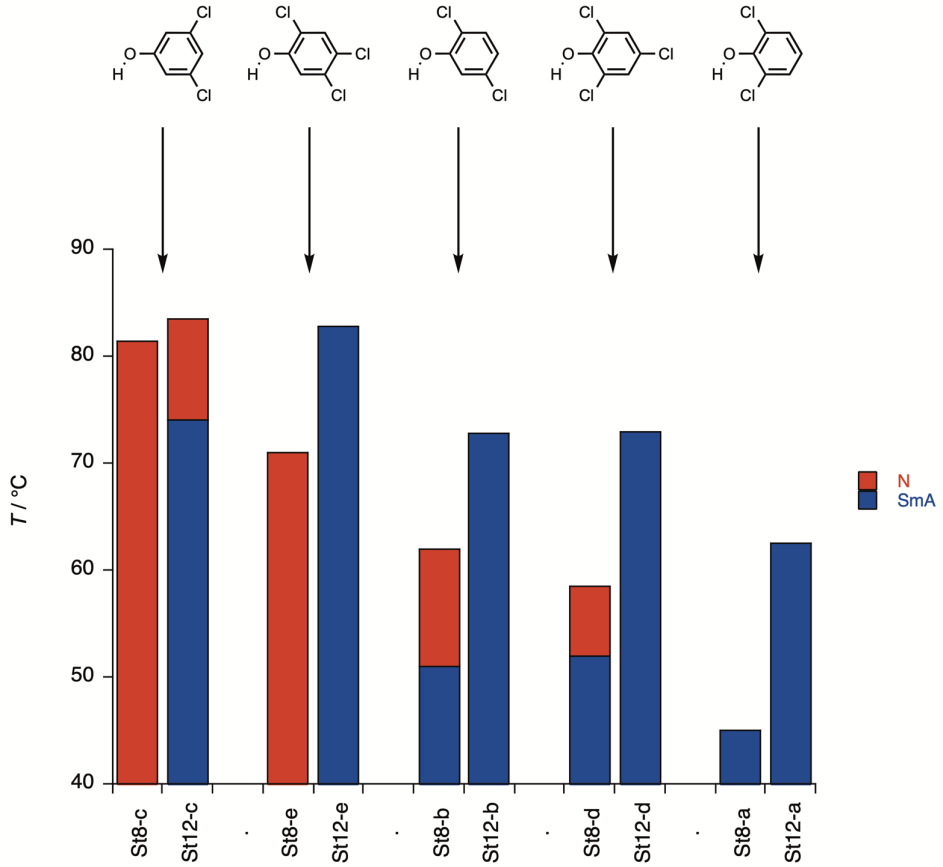

Figure S3 Clearing points of the new complexes plotted from left to right as a function of decreasing clearing point.

References

1 D. M. Huck, H. L. Nguyen, B. Donnio and D. W. Bruce, *Liq. Cryst.*, 2004, **31**, 503-507.

2 'SMART' - control software Bruker SMART Apex X-ray Diffractometer. v5.625, Bruker-AXS GMBH, Karlsruhe, Germany.

3 'SAINT+' - integration software for Bruker SMART detectors. v6.45, Bruker-AXS GMBH, Karlsruhe, Germany.

4 'SADABS' - program for absorption correction. v2.10. G. M. Sheldrick, Bruker AXS Inc., Madison, Wisconsin, USA, **2007**.

5 SHELXS-97' - program for structure solution. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, **1997**.

6 SHELXL-97' - program for the Refinement of Crystal Structures. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, **1997**.