

Electronic Supplementary Information

Photoresponsive ionic liquid crystals assembled via halogen bond: en route towards light-controllable ion transporters

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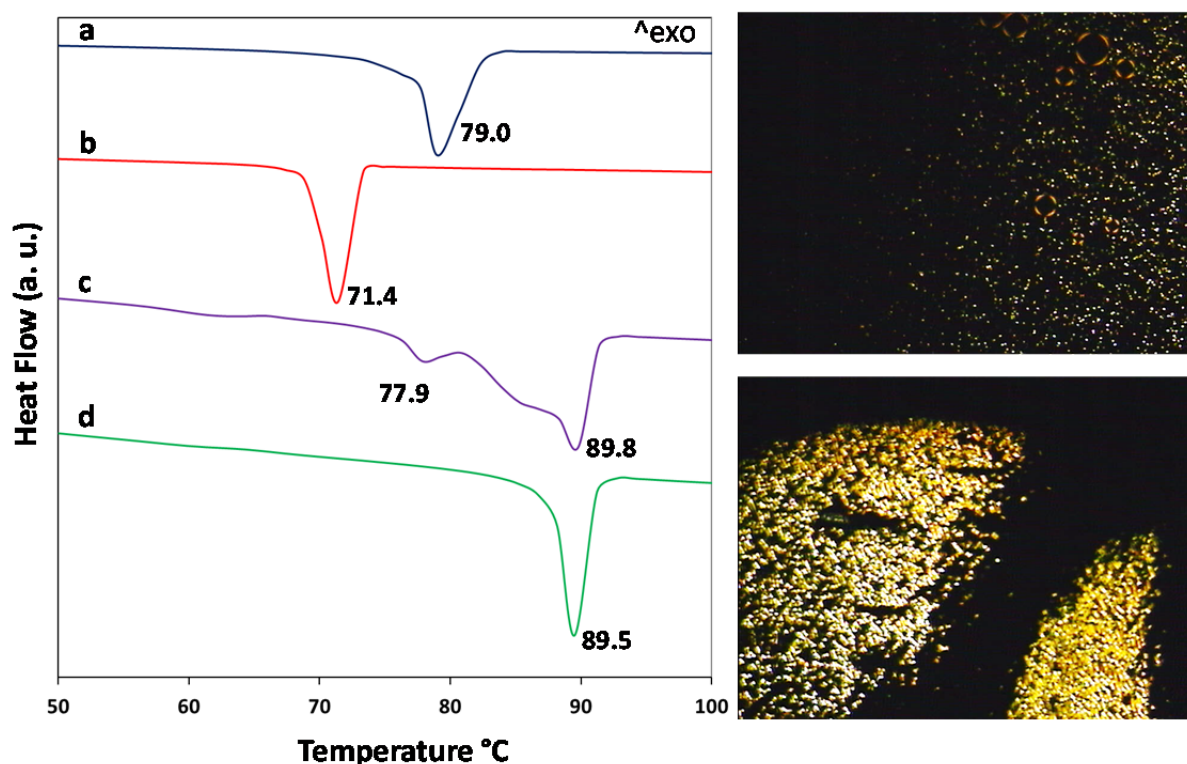


Figure 1: Left: DSC thermographs upon the first heating cycle at 10 °C min⁻¹ of: a) 1-Et-3-Me-imidazolium iodide (**1**); b) AZO_{OC10}; c) Complex **1**/AZO_{OC10} (1:1 ratio); d) Complex **1**·AZO_{OC10} (1:2 ratio). Peak maximum temperatures of each peak are indicated in the graph. Right: Optical textures of the smectic A phase observed on cooling from the isotropic state for complex **1**·AZO_{OC10} (top; T = 79,2 °C; bottom; T = 75,1 °C).

Table S1. Experimental details for **3·AZO_{OC12}** and **2·AZO_{NC1}**

Compound	3·AZO_{OC12}	2·AZO_{NC1}
Chemical Formula	$2(\text{C}_{24}\text{H}_{29}\text{F}_4\text{IN}_2\text{O}) \cdot (\text{C}_{16}\text{H}_{31}\text{N}_2)^+ \cdot (\text{I})^-$	$2(\text{C}_{14}\text{H}_{10}\text{F}_4\text{IN}_3) \cdot (\text{C}_{12}\text{H}_{23}\text{N}_2)^+ \cdot (\text{I})^-$
Formula weight	1507.11	1168.52
CCDC number		
Temperature (K)	103	103
Crystal system	Triclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁
<i>a</i> (Å)	14.9747(15)	10.406(2)
<i>b</i> (Å)	18.898(2)	7.8092(14)
<i>c</i> (Å)	25.034(3)	26.717(5)
α (°)	87.618(12)	90
β (°)	76.317(10)	92.90(2)
γ (°)	76.576(10)	90
Volume (Å ³)	6694.6(13)	2168.3(7)
<i>Z</i>	4	2
Crystal size (mm ³)	0.22 x 0.21 x 0.10	0.27 x 0.17 x 0.09
μ (mm ⁻¹)	1.47	2.24
<i>T</i> _{min} , <i>T</i> _{max}	0.607, 0.695	0.632, 0.747
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	208179, 42910, 27374	89689, 18631, 17551
<i>R</i> _{int}	0.039	0.024
(sin θ/λ) _{max} (Å ⁻¹)	0.737	0.827
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.037, 0.090, 1.02	0.02, 0.045, 1.02
No. of reflections	42910	18631
No. of parameters, No. of restraints	1503, -	536, 1
$\Delta\rho_{\text{min}}, \Delta\rho_{\text{max}}$ (e Å ⁻³)	-0.88, 3.56	-0.43, 1.25

Computer programs: Bruker APEX2, Bruker SAINT, SHELXS (Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122), SHELXL (Sheldrick, G. M. (2015). Acta Cryst. A64, 112-122), Mercury (Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). J. Appl. Cryst. 39, 453-457