Supporting Information

New cyanopyridone based luminescent liquid crystalline materials: Synthesis and characterization

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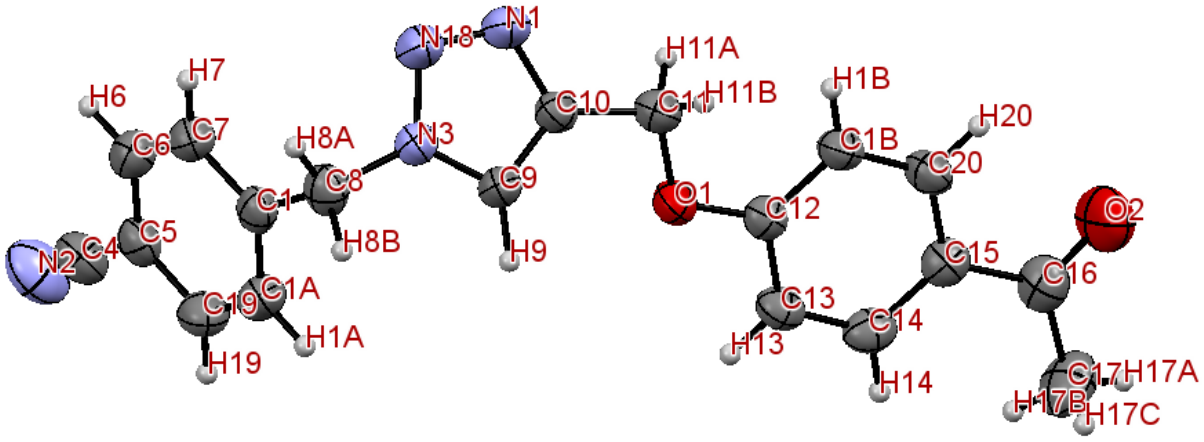

Figure S1 ORTEP diagram of **3a** with atom numbering. ORTEP diagram is drawn with 50% probability ellipsoids at 296 K.

Table S1 Crystal data and structure refinement for compound **3a**

Compound	**3a**
Formula	$C_{19}H_{16}N_4O_2$
Formula weight	332.36
CCDC number	966496
Temperature (K)	296
Crystal form	Block
Color	Colorless
Crystal system	Monoclinic
Space group	*P 21/c*
a (Å)	20.3809(14)
b (Å)	5.5940(4)
c (Å)	15.3584(11)
α (°)	90
β (°)	105.915(4)
γ (°)	90
Volume ($Å^3$)	1683.91
Z	4
Density (gcm^{-3})	1.311
μ (mm^{-1})	0.09
F (000)	696.0
$h_{min, max}$	-23,25
$k_{min, max}$	-5,6

$l_{min, max}$	-18,16
Reflections collected	11617
Independent reflections	3240
$R_{\_all}$, $R_{\_obs}$	0.1022, 0.0526
wR_{2_all}, wR_{2_obs}	0.1587, 0.1373
$\Delta\rho_{min,max}$ (e Å^{-3})	-0.23, 0.26
GOOF	0.92

2. PXRD data of 5b and 5f

Table S2 X-ray diffraction results of **5b** and **5f** in their hexagonal columnar phase

Compound	**Phase**	d_{exp}/Å	d_{theo}/Å	**Miller Indices *hk***	**Lattice Parameters (Å) Lattice Area S (Å^2) Molecular Volume V (Å^3)**
5b	Col_h at 30 °C	41.61 4.11	41.61	10 halo (*h*)	a= 48.10 Å S= 2675 Å^2 V_{cell}= 10995 Å^3 V_{mol}= 1329 Å^3 Z = 8
5f	Col_h at 30 °C	37.96 4.31	37.96	10 halo (*h*)	a= 44 Å S= 1666 Å^2 V_{cell}= 7180 Å^3 V_{mol}= 1267 Å^3 Z = 6

Note: The notations d_{exp} and d_{theo} are experimental and theoretical diffraction spacings, respectively. d_{theo} is deduced from the lattice parameter a (Col_h) from the following mathematical expression: $d_{theo} = [2/(\sqrt{3}N_{hk})].[\sum_{hk} d_{hk}\sqrt{(h^2+k^2+hk)}]$, where N_{hk} is the number of *hk* reflections observed for the Col_h phase. S is the lattice area, given by: $S = (a^2\sqrt{3})/2$ Cell volume, $V_{cell} = h.S$

(where h is the thickness of hexagonal stratum). The molecular volume is defined as $V_{mol} = M/(\delta \times 0.6022)$, where M is molecular weight; $V_{CH2}(T) = 26.5616+0.02023T$ (T in °C, T_0=25°C); density $\delta = V_{CH2}(T_0)/ V_{CH2}(T)$; the aggregation number or the number of molecular equivalents per stratum of column $Z = V_{cell}/V_{mol}$. I represents the intensity of reflections (VS: very strong, S: strong, M: medium, VW: very weak, br: broad); hk are the indexations of the reflections corresponding to the Col_h phase.