Support Information

Synthesis and characterization of some novel tetrazol liquid crystals.

Muhammad Tariq,1,2 Shahid Hameed,2 Ivan H. Bechtold3 Adailton J. Bortoluzzi4 and Aloir A. Merlo*1

1. Institute of Chemistry, UFRGS, Porto Alegre, RS, Brazil.
2. Department of Chemistry, Quaid-i-Azam University, Islamabad-45320, Pakistan.
3. Department of Chemistry, UFSC, Florianópolis, SC, Brazil.
4. Department of Physics, UFSC, Florianópolis, SC, Brazil.

Figure S1. Schlieren texture observed for nematic mesophase upon cooling at 79°C for 5g.
Figure S2. (a), (b) and (c) Schlieren texture observed during the mesophase transition from nematic to smectic mesophase upon cooling at ca 71°C for 5g.
Figure S3. DSC TA Q2000 at 10 °/min for 5a.

Figure S4. DSC TA Q20 at 5 °/min for 5a.
Figure S5. DSC TA Q20 at 5 °/min for 5b.

Figure S6. DSC TA Q20 at 5 °/min for 5c.
**Figure S7.** DSC TA Q2000 at 10 °C/min for 5d.

**Figure S8.** DSC TA Q2000 at 2 °C/min for 5d.
Figure S9. DSC TA Q2000 at 5 °C/min and 2 °C/min for 5e (on November, 22th).

Figure S10. DSC TA Q2000 at 5 °C/min for 5e (on May, 17th)
Figure S11. DSC TA Q2000 at 10 °/min for 5f.

Figure S12. DSC TA Q2000 at 2 °/min for 5f.
Figure S13. DSC TA Q2000 at 3 °/min for 5g.

Figure S14. DSC TA Q20 at 1 °/min for 5h.
Figure S15. TGA/DTG curve for 5c in the temperature range 20 – 600 °C. A derivative weight loss curve has been added to show the point at which weight loss is most apparent.
SUPPORT INFORMATION

X-Ray data

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1. Single Crystal X-ray Diffraction

1.1. Compound 5a

Table 1. Crystal data and structure refinement for 5a.

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<tr>
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<td>Pī</td>
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<tr>
<td></td>
<td>b = 10.9801(3) Å, (\beta= 72.7700(10)^\circ)</td>
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<tr>
<td></td>
<td>c = 13.8034(4) Å, (\gamma= 76.798(2)^\circ)</td>
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<tr>
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<td>Refinement method</td>
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Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C
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Table 2. Bond lengths [Å] and angles [°] for 5a.

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<th>Bond</th>
<th>Length [Å]</th>
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N(1)-C(1)-C(11)  123.90(11)  C(25)-C(24)-C(23)  120.42(12)
N(4)-C(1)-C(11)  123.92(12)  C(26)-C(25)-C(24)  119.08(12)
O(2)-C(2)-O(1)  122.38(12)  C(26)-C(25)-H(25)  120.5
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C(23)-C(22)-C(21)  120.62(12)  C(35)-C(34)-H(34A)  108.8
C(23)-C(22)-H(22)  119.7  C(33)-C(34)-H(34A)  108.8
C(21)-C(22)-H(22)  119.7  C(35)-C(34)-H(34B)  108.8
C(22)-C(23)-C(24)  119.75(12)  C(33)-C(34)-H(34B)  108.8
C(22)-C(23)-H(23)  120.1  H(34A)-C(34)-H(34B)  107.7
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Table 3. Torsion angles [°] for 5a.

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1.2. Compound 5f
Table 4. Crystal data and structure refinement for 5f.

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Table 5. Bond lengths [Å] and angles [°] for 5f.

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N(2)-C(31)-C(32) 113.2(3)  C(38)-C(37)-C(36) 113.1(4)
N(2)-C(31)-H(31A) 108.9  C(38)-C(37)-H(37A) 109.0
C(32)-C(31)-H(31A) 108.9  C(36)-C(37)-H(37A) 109.0
N(2)-C(31)-H(31B) 108.9  C(38)-C(37)-H(37B) 109.0
C(32)-C(31)-H(31B) 108.9  C(36)-C(37)-H(37B) 109.0
H(31A)-C(31)-H(31B) 107.8  H(37A)-C(37)-H(37B) 107.8
C(31)-C(32)-C(33) 109.5(3)  C(37)-C(38)-C(39) 112.5(4)
C(31)-C(32)-H(32A) 109.8  C(37)-C(38)-H(38A) 109.1
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C(35)-C(36)-C(37) 112.5(3)  C(44)-C(43)-C(42) 110.8(3)
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**Molecule 2**

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Table 6. Torsion angles [°] for 5f.

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