Electronic supplementary information for:

Novel selenoesters fluorescent liquid crystalline exhibiting a rich phase polymorphism.

Daniel S. Rampon,^a Fabiano S. Rodembusch,^a Juliana M. F. M. Schneider,^a Ivan H. Bechtold,^b Paulo F. B. Gonçalves,^c Aloir A. Merlo^{a,*} and Paulo H. Schneider^{a,*}

^a Instituto de Química, Universidade Federal do Rio Grande do Sul, UFRGS, C.P. 15003, 9150-970, Porto Alegre, Brazil.

^b Departamento de Física, Universidade Federal de Santa Catarina – UFSC, 88040-900 Florianópolis-SC, Brazil

^c Instituto de Química, Centro Universitário La Salle. Av. Victor Barreto, 2288. Centro. 92010-000, Canoas, RS -Brasil

*Corresponding author. FAX +55 51 3308 7304; Tel +55 51 3308 6286; e-mail: paulos@iq.ufrgs.br

Contents

1. NMR spectra of compounds	S-2
2. DSC thermograms	S-14
3. Microscopic Analysis	S-16
4. XRD Spectrum of compound 4b	S-19

NMR Spectra of compounds:



Figure 1. ¹H NMR spectrum of compound 1-bromo-4-octyloxybenzene (CDCl₃, 300 MHz).



Figure 2. ¹³C NMR spectrum of compound 1-bromo-4-octyloxybenzene (CDCl₃, 75 MHz).



Figure 3. ¹H NMR spectrum of compound **4-(4-octyloxyphenyl)-2-methylbut-3-yn-2-ol** (CDCl₃, 300 MHz).



Figure 4. ¹³C NMR spectrum of compound 4-(4-octyloxyphenyl)-2-methylbut-3-yn-2-ol (CDCl₃, 75 MHz).



Figure 5. ¹H NMR spectrum of compound Methyl-4-(4-octyloxyphenylethynyl)benzoate (CDCl₃, 300 MHz).



Figure 6. ¹³C NMR spectrum of compound Methyl-4-(4-octyloxyphenylethynyl)benzoate (CDCl₃, 75 MHz).



Figure 7. ¹H NMR spectrum of compound 4-[4-(Octyloxyphenylethynyl)]benzoic acid 3 (DMSO-d6, 300 MHz).



Figure 8. ¹³C NMR spectrum of compound 4-[4-(Octyloxyphenylethynyl)]benzoic acid 3 (DMSO-d6, 75 MHz).



Figure 9. ¹H NMR spectrum of compound Methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate 4a (CDCl₃, 300 MHz).



Figure 10. ¹³C NMR spectrum of compound Methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate 4a (CDCl₃, 75 MHz).



Figure 11. ¹H NMR spectrum of compound **4-Octyloxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate 4b** (CDCl₃, 300 MHz).

•



Figure 12. ¹³C NMR spectrum of compound 4-Octyloxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate 4b (CDCl₃, 75 MHz)

DSC thermograms:



Thermograms set for compounds **4a-b** on heating at 10°C min⁻¹.

Figure 13. Thermogram for compound Methoxyphenyl-4-[(4-octyloxyphenyl)ethynyl]benzoselenoate 4a.



Figure 14. Thermogram for compound 4-Octyloxyphenyl-4-[(4-octyloxyphenyl)ethynyl]benzoselenoate 4b.

Microscopic Analysis:

Polarized-light optical microscopy analysis for compound **4-Octyloxyphenyl-4-[(4-octyloxyphenyl)ethynyl]-benzoselenoate 4b**.



Figure 15. Planar thread-like nematic texture occurring at 164 °C.



Figure 16. Schlieren texture grainy at 144 °C of the smectic C phase.



Figure 17. Schlieren type texture of smectic I phase with loops of disclination lines at 105 ° C.



Figure 18. Paramorphotic mosaic texture of the smectic I at 82.0 °C.



Figure 19. Mosaic texture of the smectic I at 100.5°C.



Figure 20. Mosaic texture of the smectic X at 58.0 °C.



Figure 21. XRD spectrum of compound 4b in solid state at 30 °C.