

Supporting Information

Nonlinear optical thin film device from a chiral octopolar phenylacetylene liquid crystal

Laura de Vega, Sijn van Cleuvenbergen, Griet Depotter, Eva M. Garcia-Frutos, Berta Gómez-Lor, Ana Omenat, Rosa M. Tejedor, José Luis Serrano, Gunther Hennrich,^{*} Koen Clays^{*}

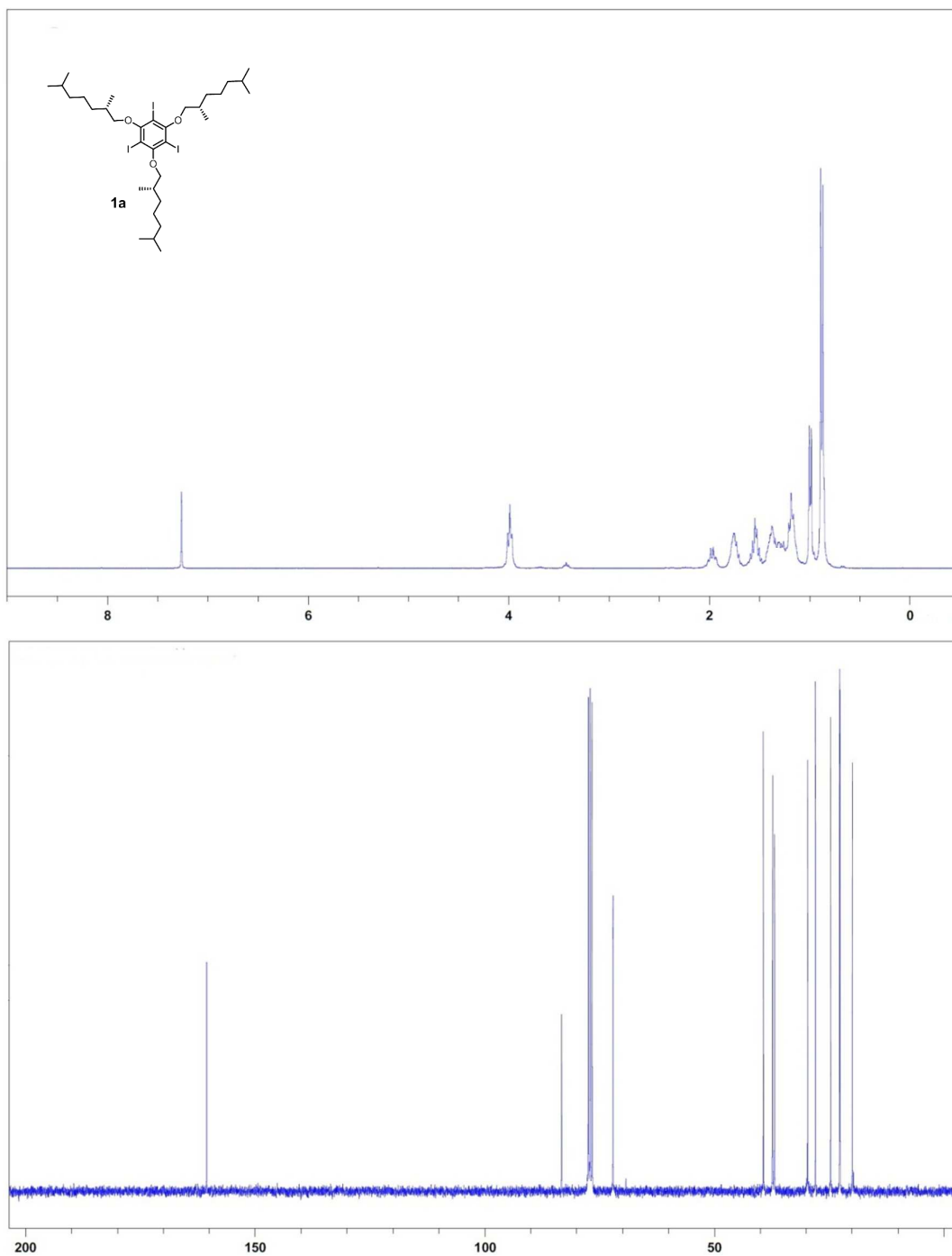
Contents.

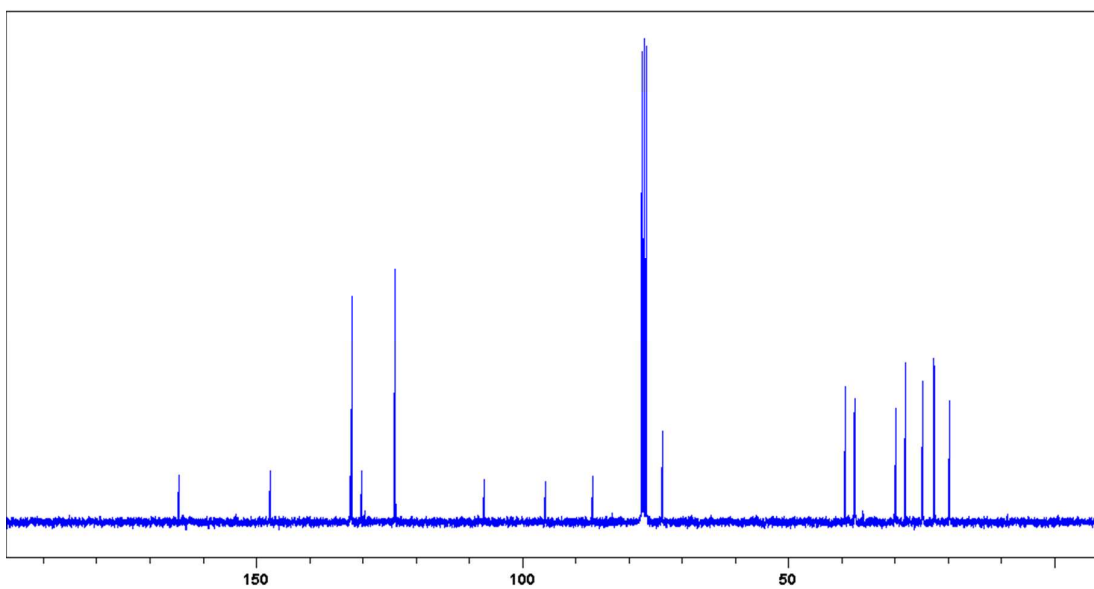
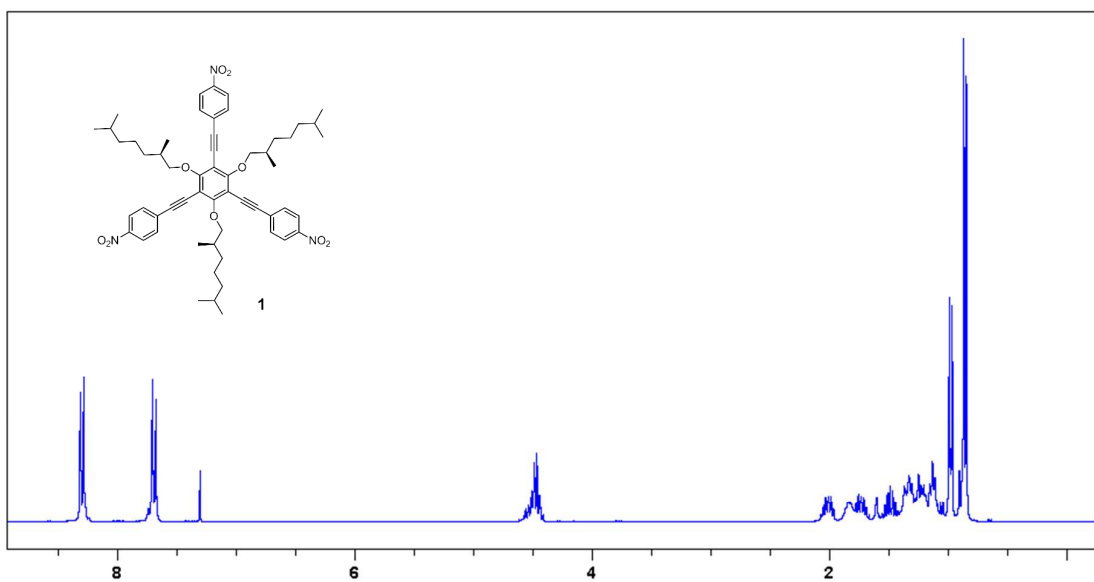
1. General methods: p.2.
2. ¹H and ¹³C NMR spectra for **1a**, **1**, **2**, **4**, **5**, **6** p3 – 8.
3. CD spectra of thin films of **1** at different temperatures: p9 – 12.
4. References: p12.

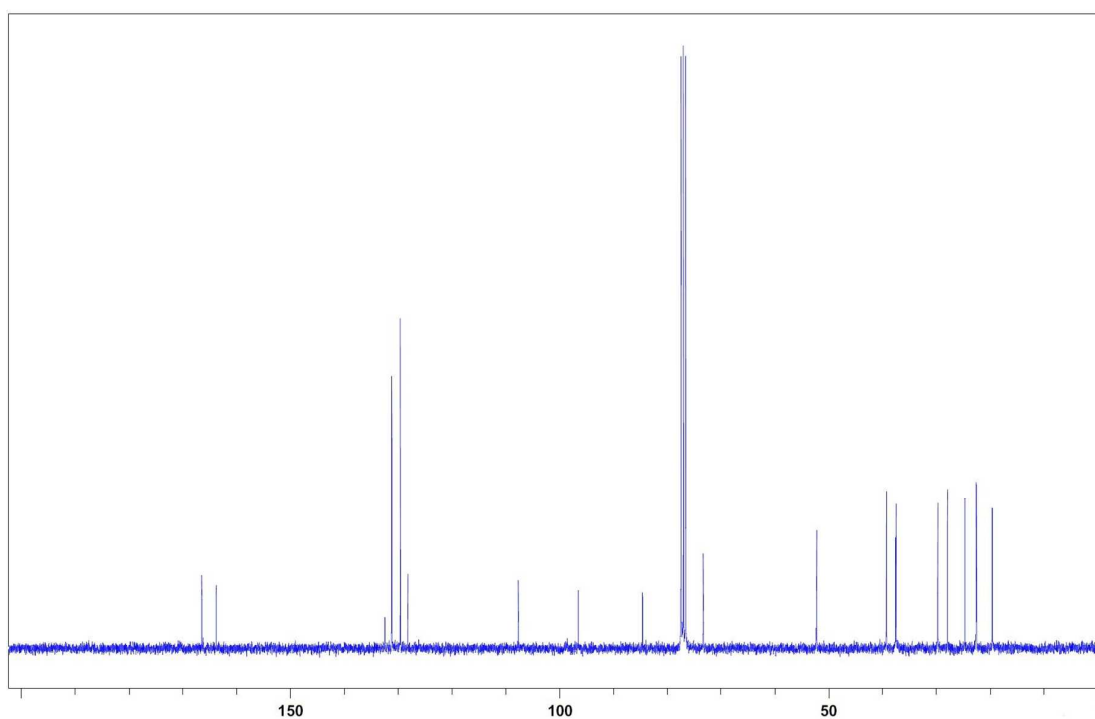
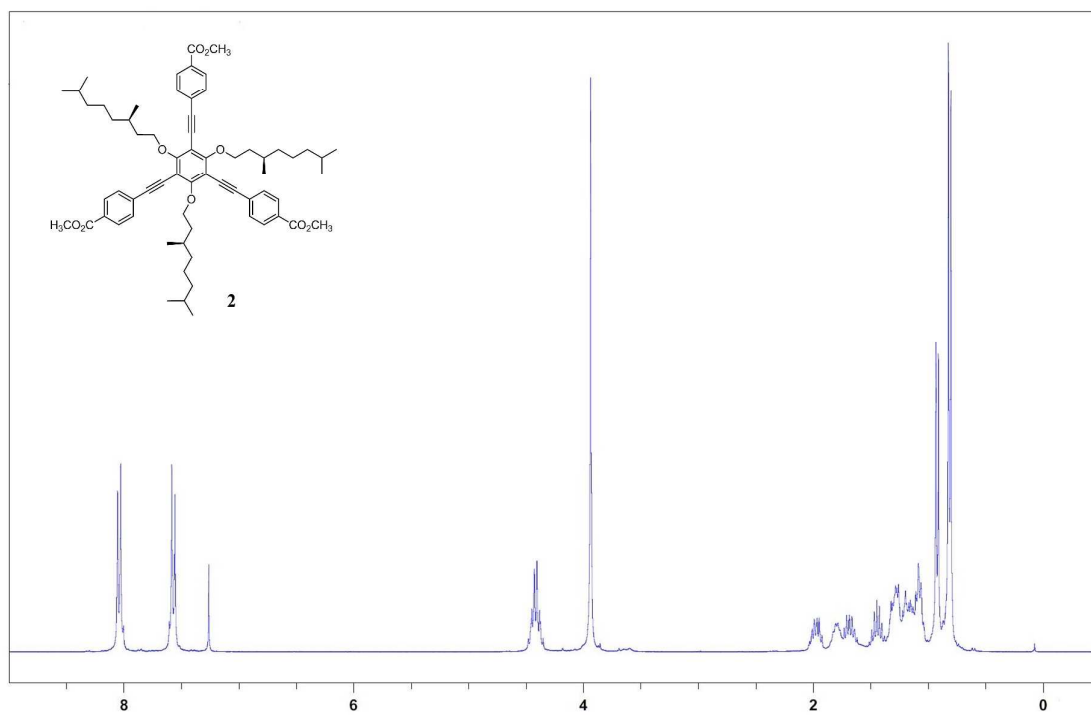
1. General methods.

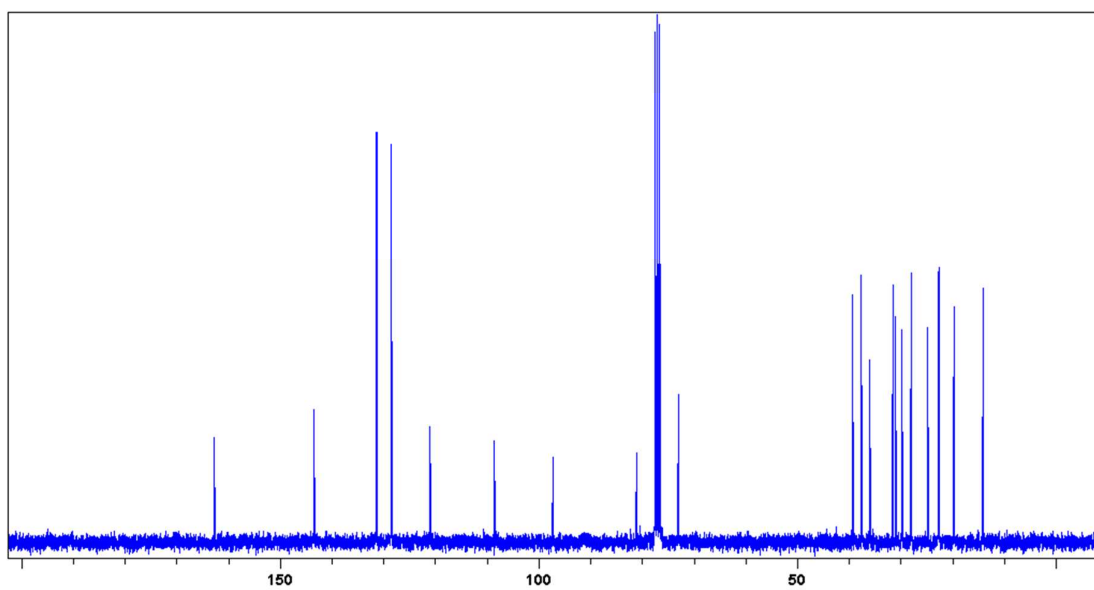
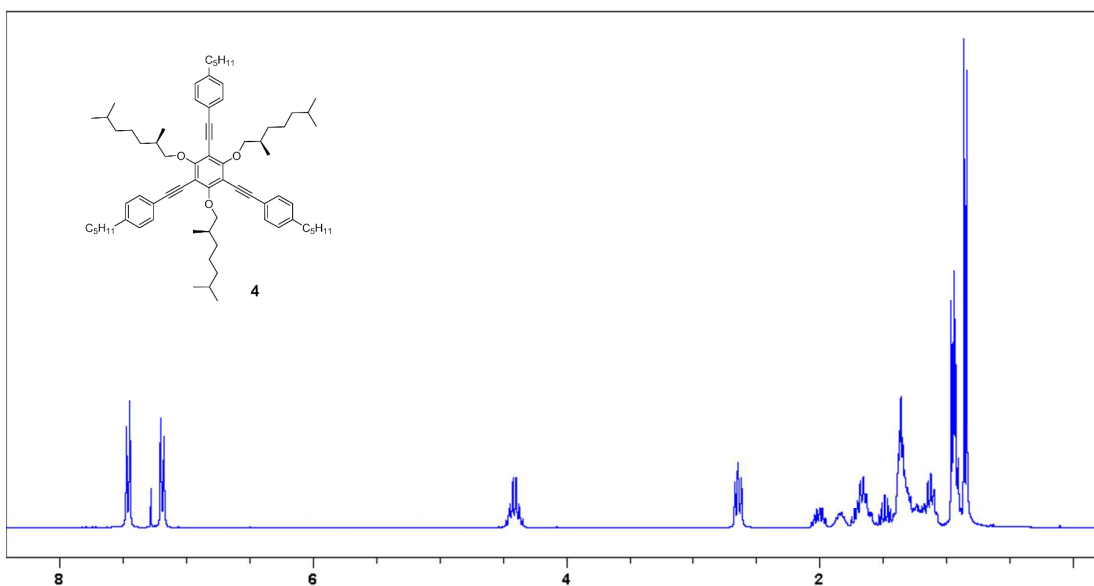
All solvents and reagents were used as purchased without further purification. ^1H and ^{13}C NMR spectra were recorded in deuterated chloroform (deuteration grade > 99.80%) with the solvent signal serving as internal standard. For the HRMS measurements a TOF analyzer has been used. Mesophase analysis was performed using a hot stage and a polarizing microscope equipped with a digital camera. Transition temperatures and enthalpies were obtained by differential scanning calorimetry at heating and cooling rates of 10 °C/min. The apparatus was previously calibrated with indium (156.6 °C, 28.44 J/g). Powder X-ray diffraction patterns were obtained using a pinhole camera operating with a point focused Ni-filtered Cu-K α beam. The sample was held in glass capillaries (0.9 and 1 mm diameter). For the VCD spectra, compound **1** was held between two BaF₂ windows and placed onto a hot stage adapted to the sample compartment of the infrared spectrophotometer. The maximum absorbance of the sample was 0.9 in the isotropic state. The mesomorphic state was obtained upon cooling of the isotropic state. The resolution was 4 cm⁻¹ and the acquisition time was 60 minutes. In order to eliminate the possible linear effects of the anisotropic samples the VCD spectra were calculated by averaging over four VCD spectra measured in selected sample orientation.¹

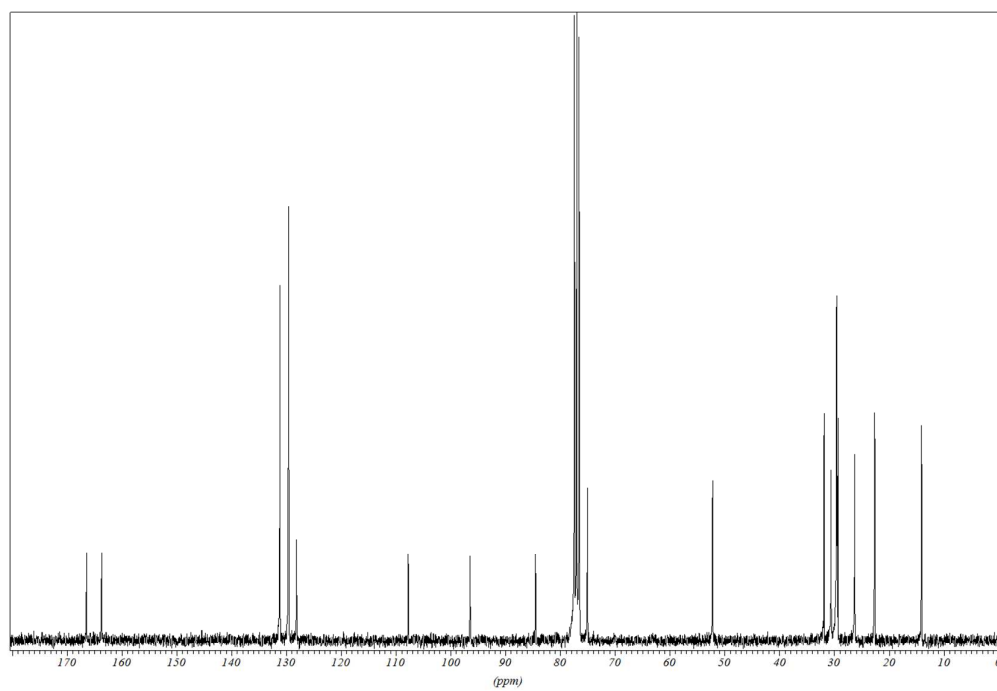
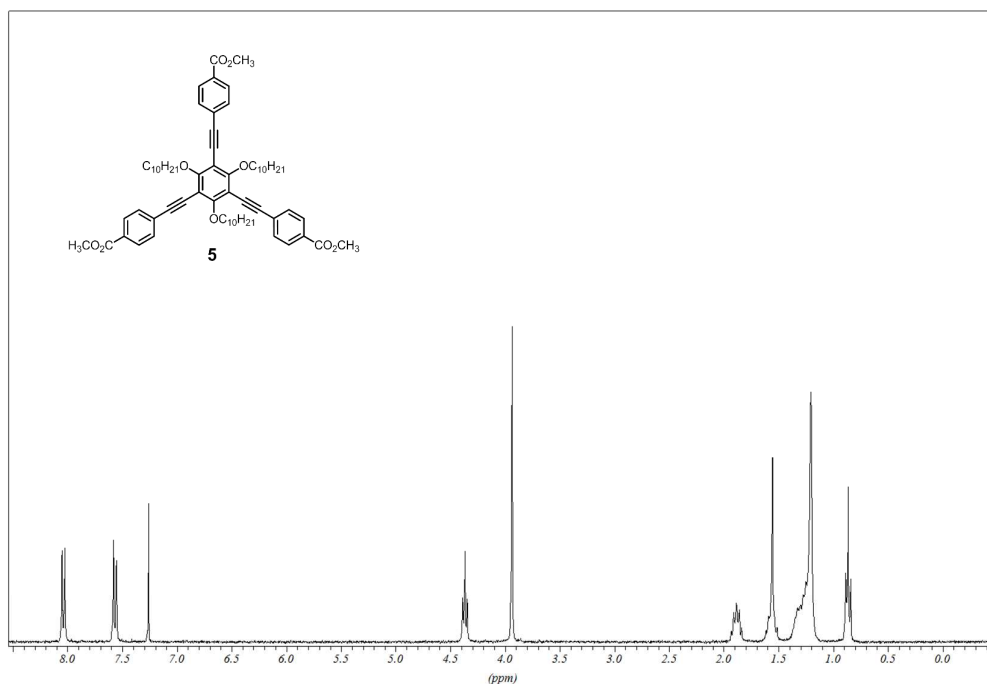
2. ^1H and ^{13}C NMR spectra of **1a**, **1**, **2**, **4**, **5**, **6**, **7a** and **7** in CDCl_3 (99.89 %), referenced to residual CHCl_3 .

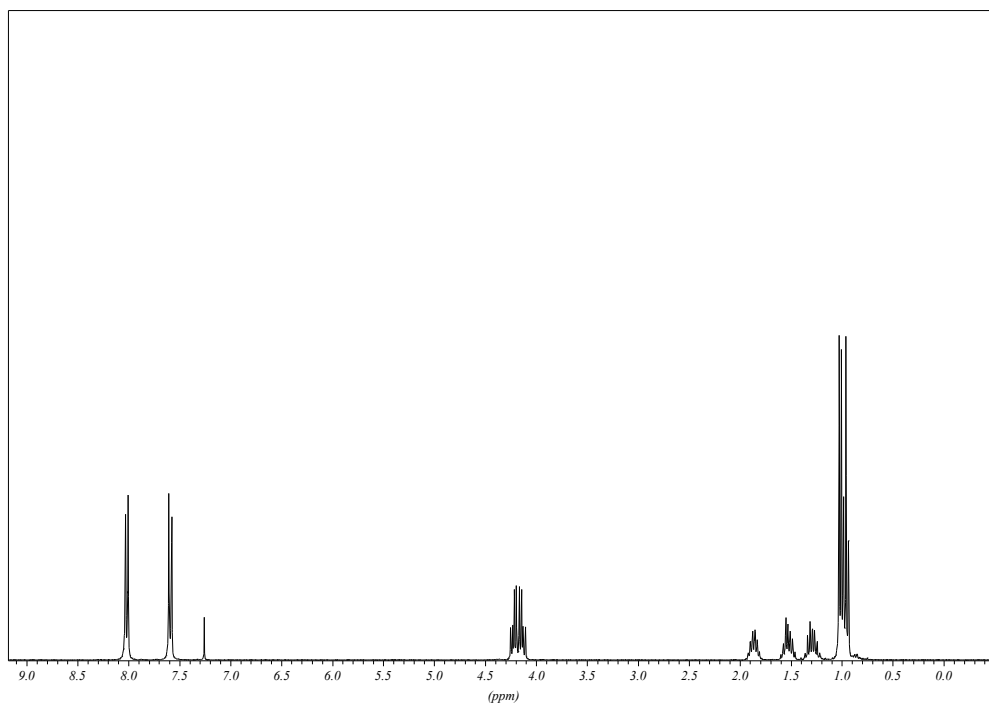
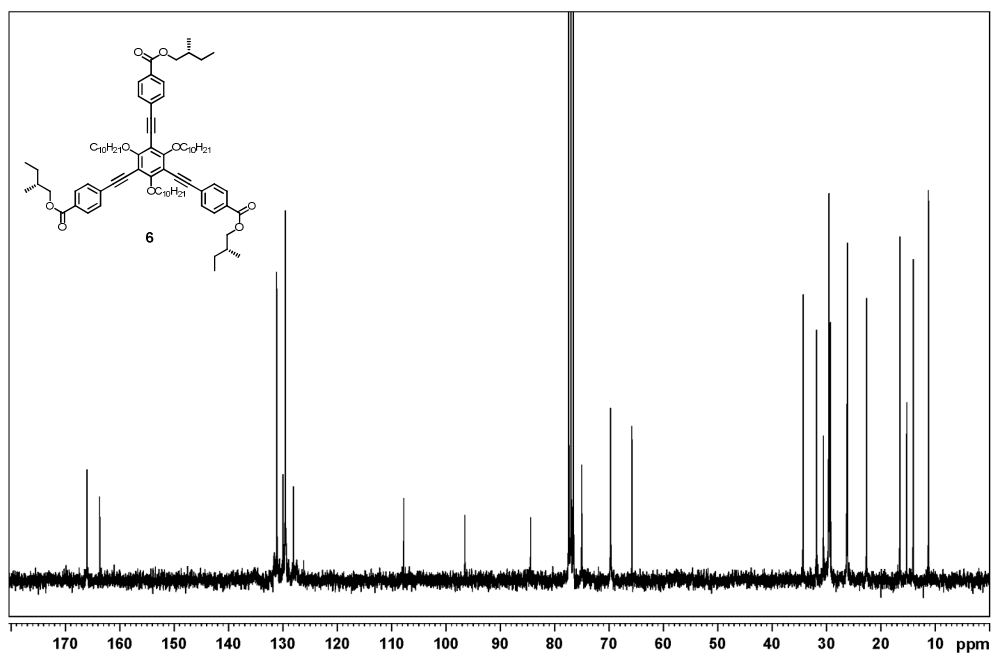








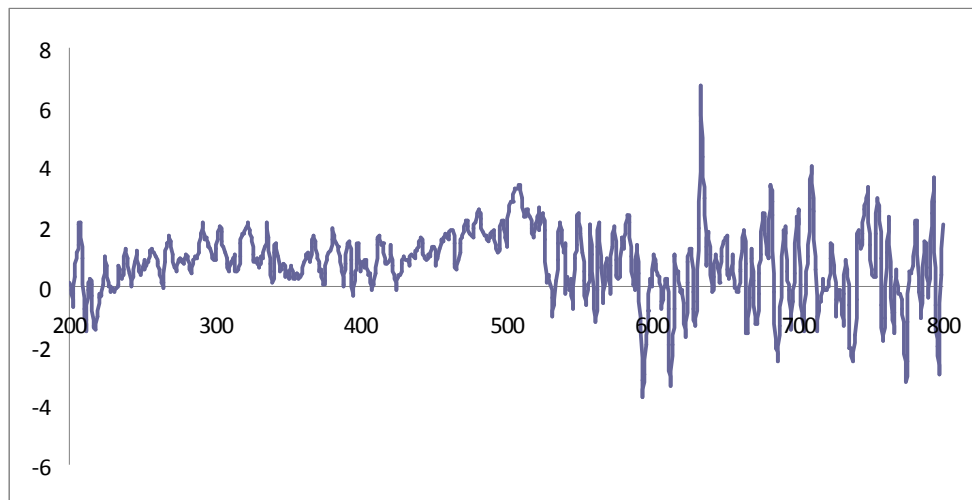




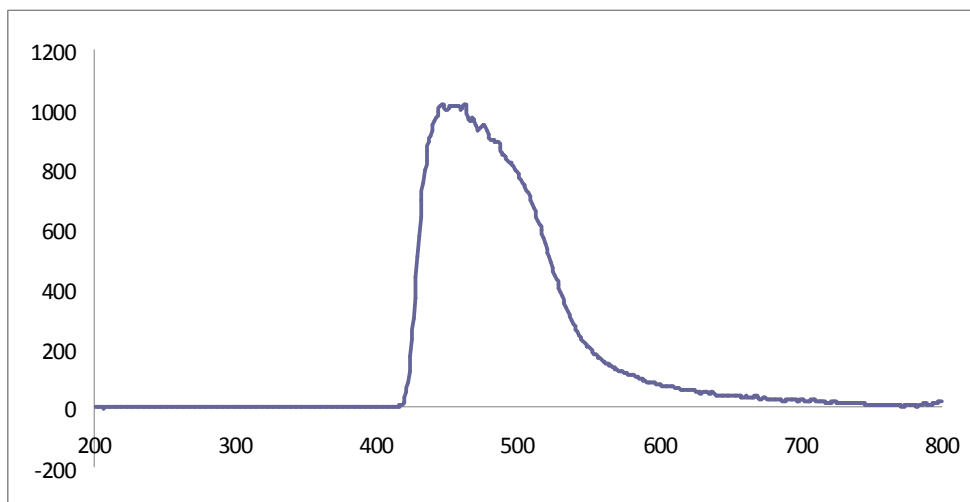
3. CD spectroscopy of 1.

1st cooling scan, measurement at the indicated temperatures.

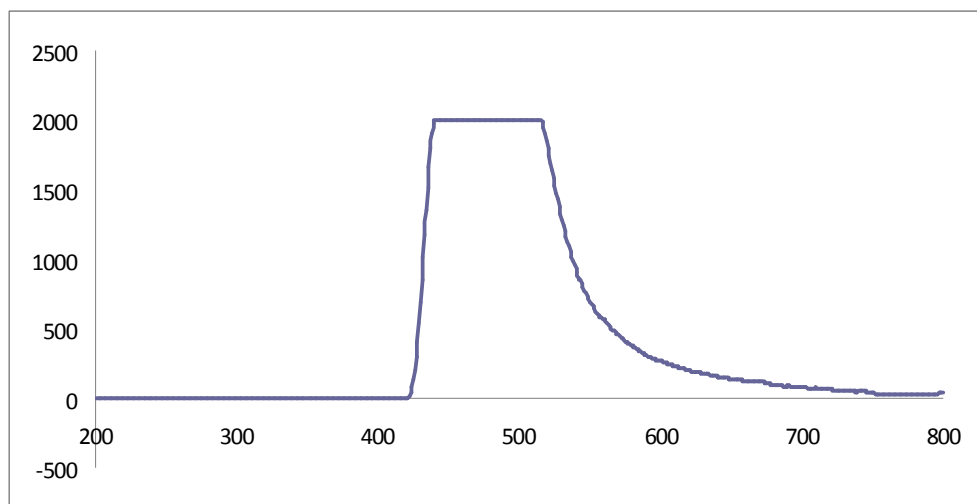
98°C



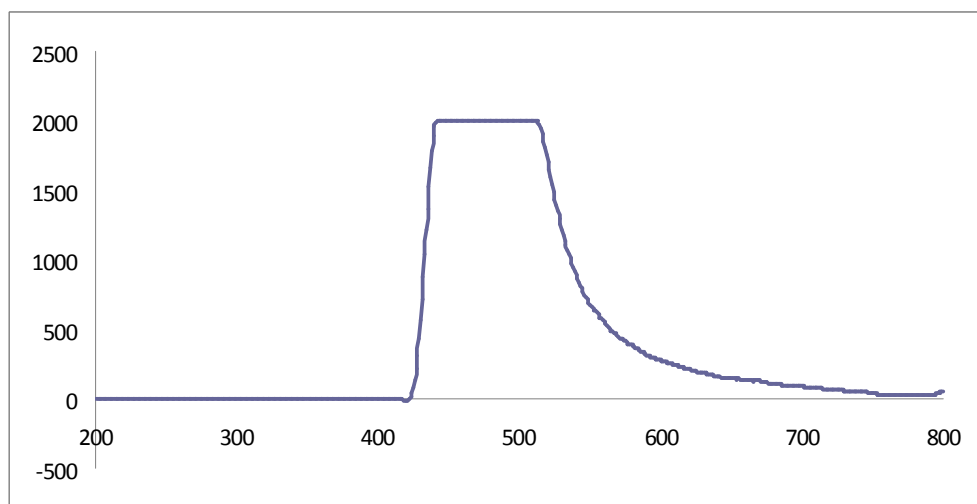
95°C



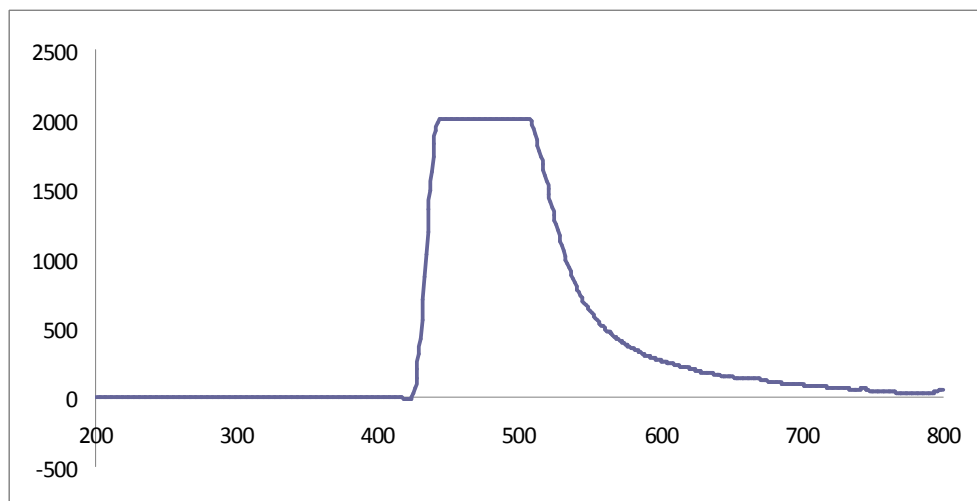
90°C



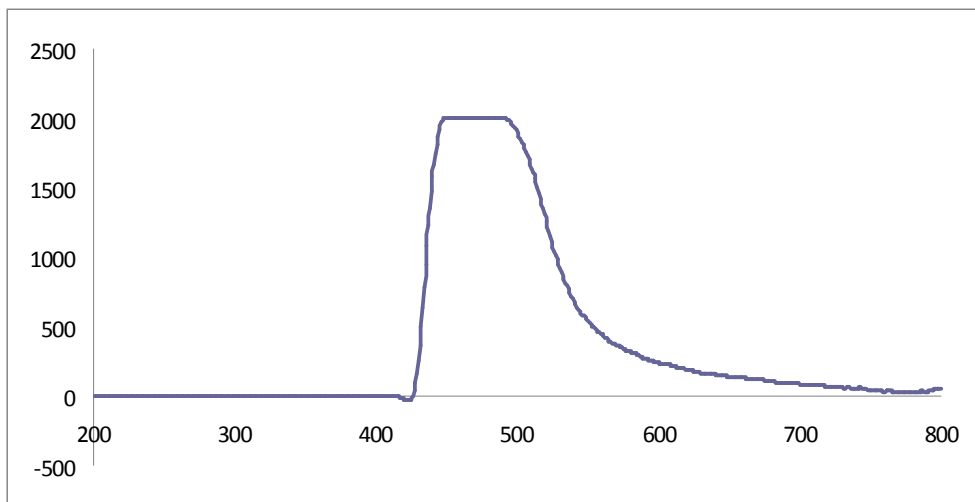
85°C



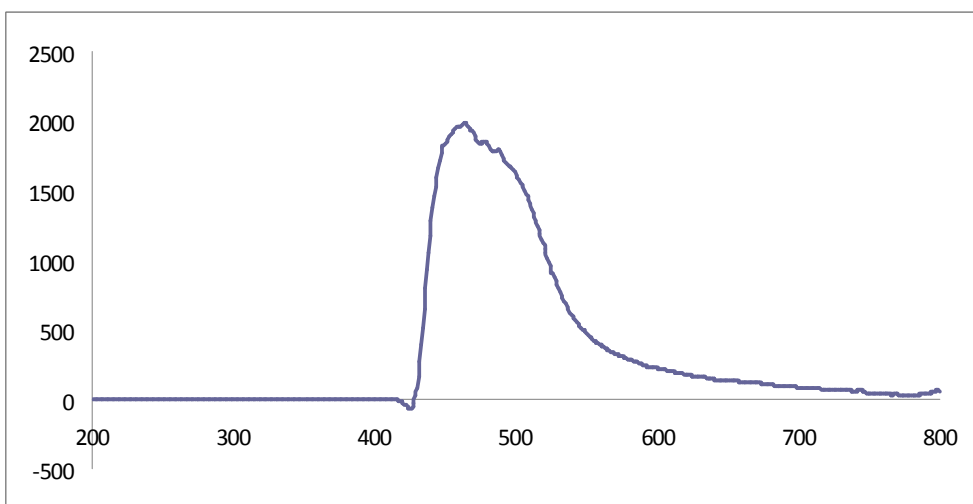
80°C



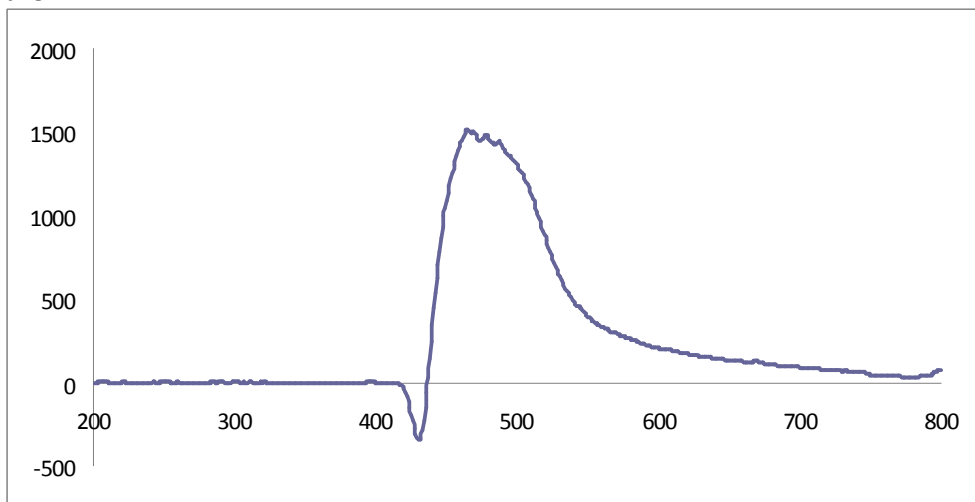
75°C



70°C

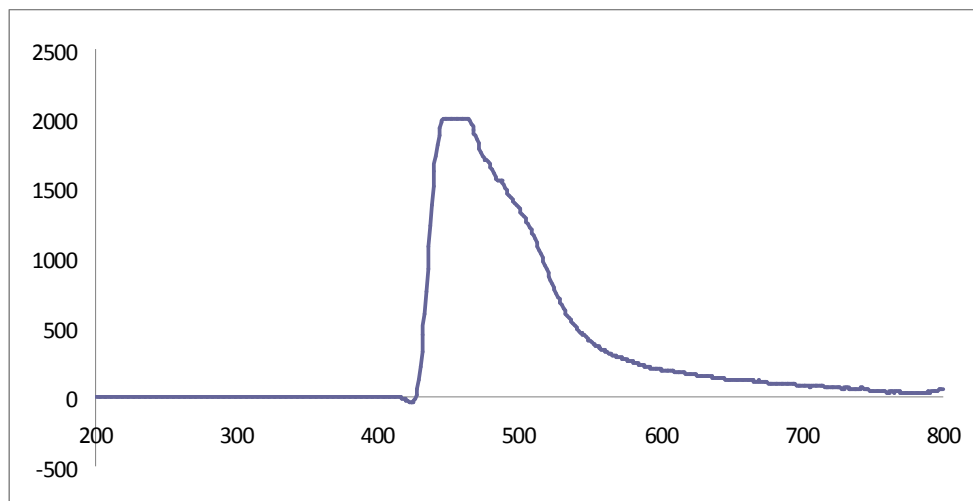


60°C

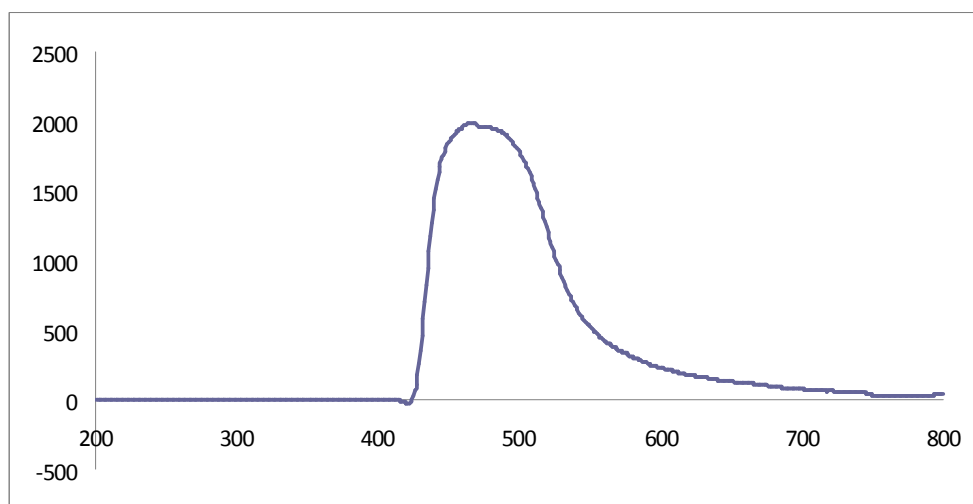


2nd heating scan.

70°C



80°C



4. References

1. C. Merten T. Kowalik, A. Hartwig, *Appl. Spectrosc.* **2008**, 62, 901- 905.