Exploring the Mesophase and Optical Behavior of Novel Furan-Based Chalcone Liquid Crystals with Ester/Azo Linkages

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SUPPORTING INFORMATION

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1. Materials

The chemicals and reaction solvents, 4-benzyloxyphenol, 1-bromododecane, 10% Pd/C, THF, 4-formylbenzoic acid, DCC, DMAP, $NaClO_2$, $NaH_2PO_4.H_2O$, t-BuOH, ethyl 4-aminobenzoate, $NaNO_2$, HCl, phenol, ethanol, sodium hydroxide, 5-bromo-2-furaldehyde, 4-hydroxyacetophenone, potassium hydroxide, 2-butanone, dichloromethane and chloroform were purchased from Sigma-Aldrich and used without further purification.

Reactions were monitored by thin layer chromatography (TLC) on aluminium plates coated with silica gel 60 F254 Merck. Column chromatography on silica gel was performed over Merck silica gel 60 (pore size 60 Å, 0.040-0.063 mm particle size).

2. Instrumentation

^{1}H-NMR spectra were recorded at room temperature in deuterated dimethylsulfoxide (DMSO-d_6) solution for compound **8** and in deuterated chloroform ($CDCl_3$) solution for compounds **CEE** and **CEA** on a Bruker 500 MHz spectrometer with tetramethylsilane as internal standard.

Olympus BX-53 polarizing optical microscope equipped with a Linkam LTS420 hot stage and control unit (Linkam T96 with LinkPad) was used to determine the thermal/mesomorphic behavior and optical textures of novel furan-based chalcone derivatives (**CEE** and **CEA**). DSC thermograms of compounds were recorded on a Netzsch DSC 3500 Sirius with a heating and cooling rate of 10 ˚C min^{-1} in a nitrogen atmosphere. Aluminium pans and 5 mg sample amounts were used for DSC measurements.

The thermogravimetric analysis (TGA) was performed by PerkinElmer, Diamond TG/DTA – Seiko Instruments SII, Exstar 6300 TG/DTA under nitrogen atmosphere at a temperature rate of 10 ˚C min^{-1} ranging from 20 to 700 ˚C.

3. Spectral Data (^{1}H-NMR and ^{13}C-NMR (APT) Spectra)

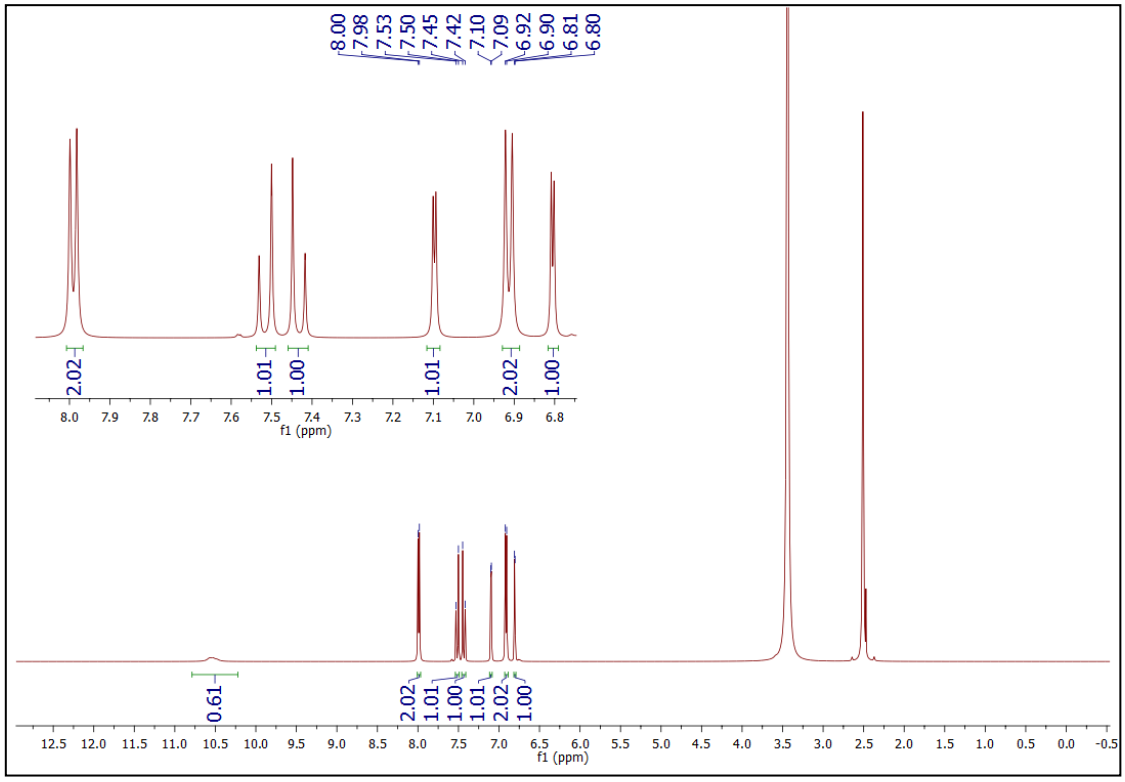

Figure S1. ^{1}H-NMR spectrum of chalcone derivative **8**.

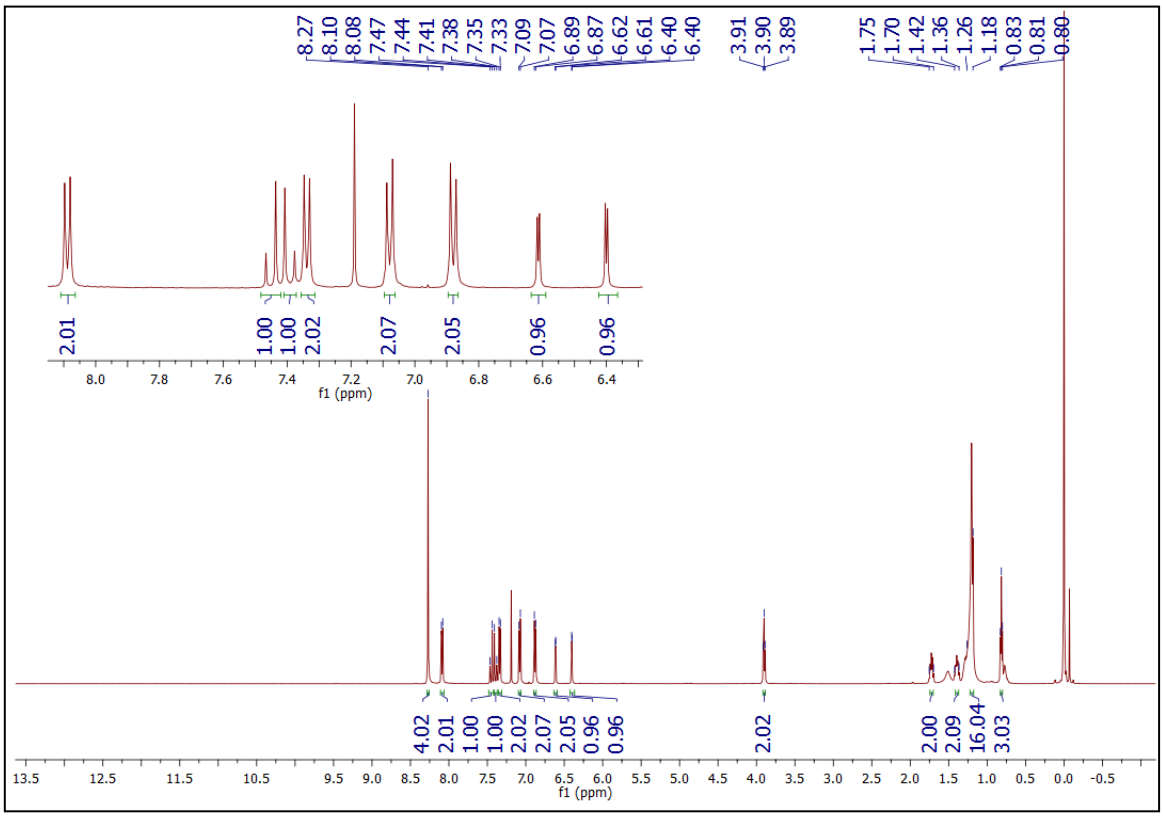

Figure S2. ^{1}H-NMR spectrum of **CEE**.

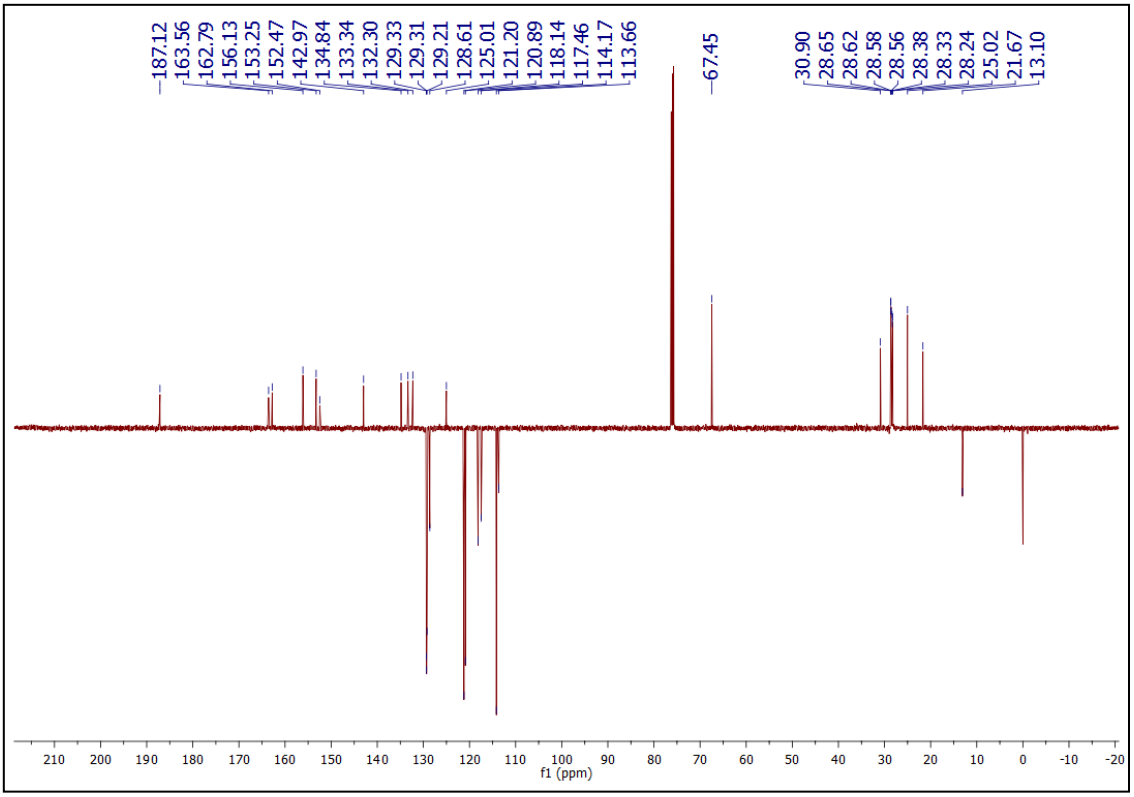

Figure S3. ^{13}C-NMR spectrum of **CEE**.

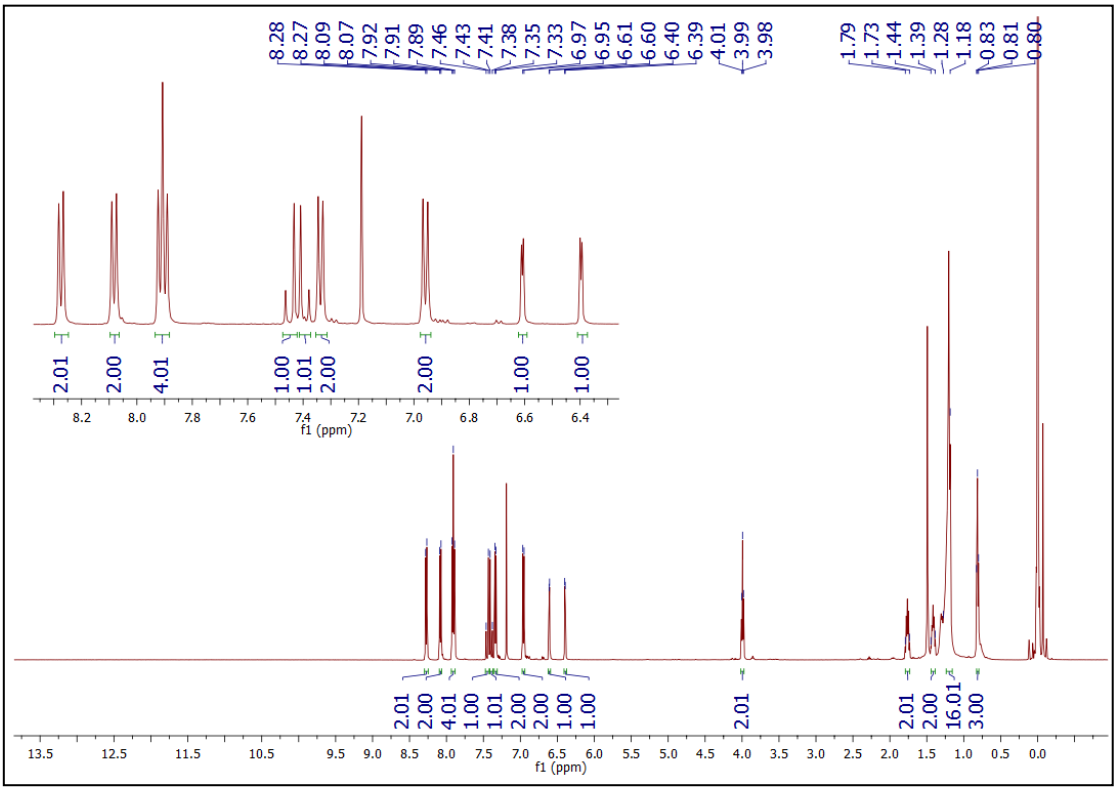

Figure S4. ^{1}H-NMR spectrum of **CEA**.

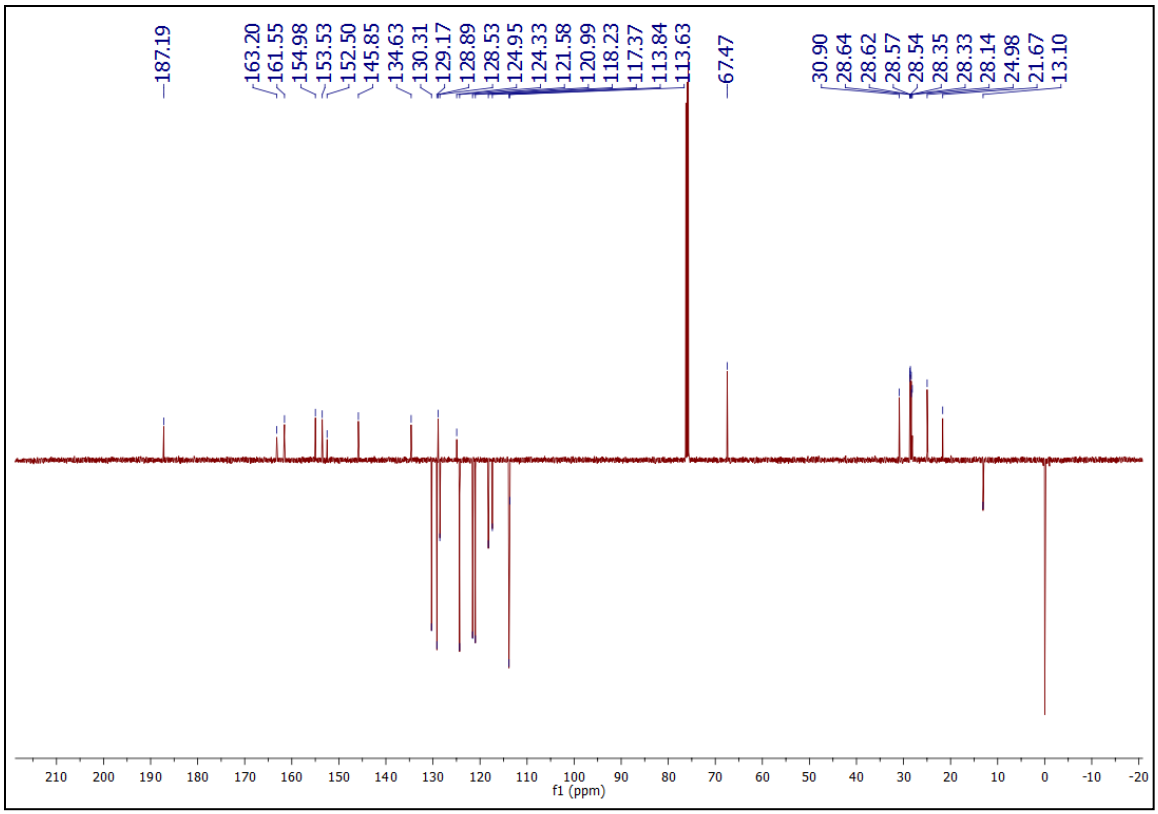

Figure S5. ^{13}C-NMR spectrum of **CEA**.

4. Thermal Behaviour (1st Heating DSC Curves)

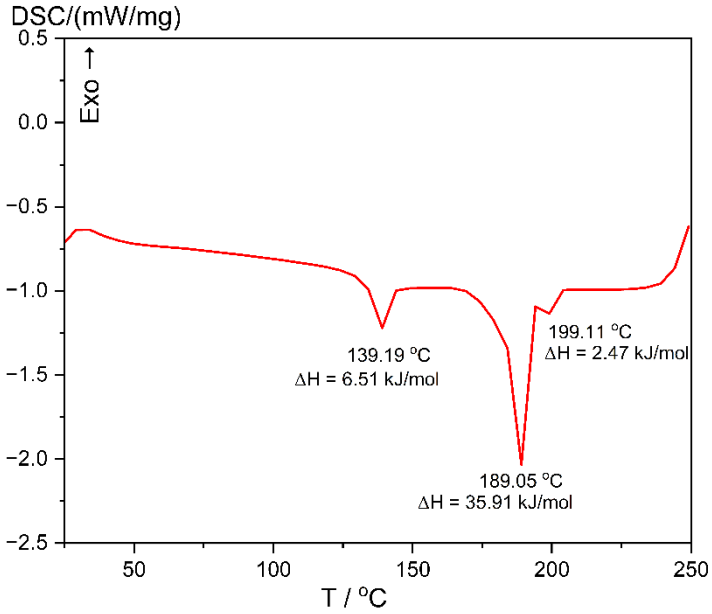

Figure S6. DSC thermogram of **CEE** on 1st heating (10 °C min^{-1}).

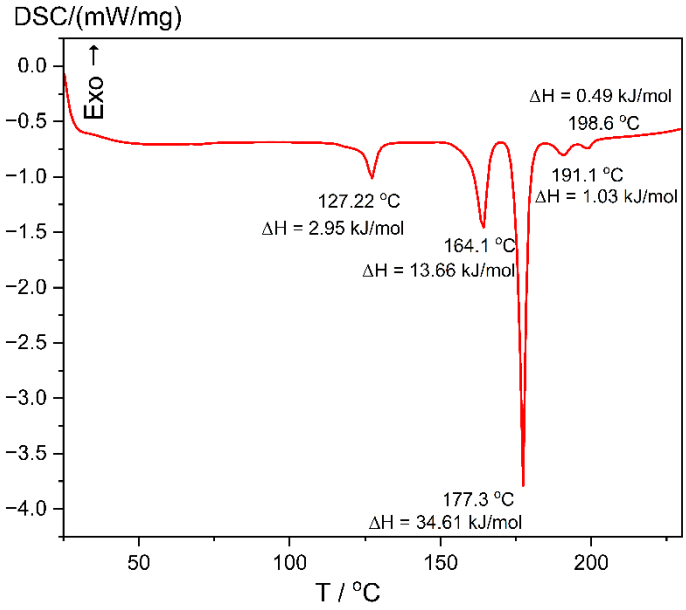

Figure S7. DSC thermogram of **CEA** on 1st heating (10 °C min^{-1}).