

Solid state photodimerisation of tetrathiafulvalene derivatives bearing carboxylate and carboxylic acid substituents

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Supporting information

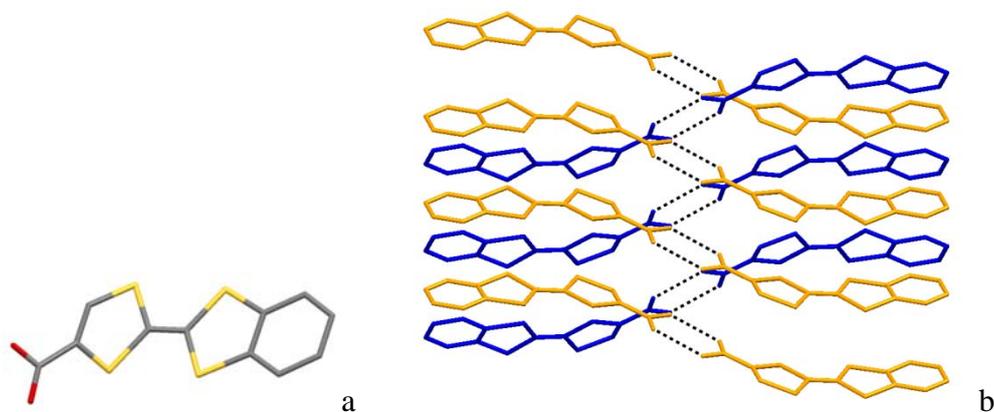
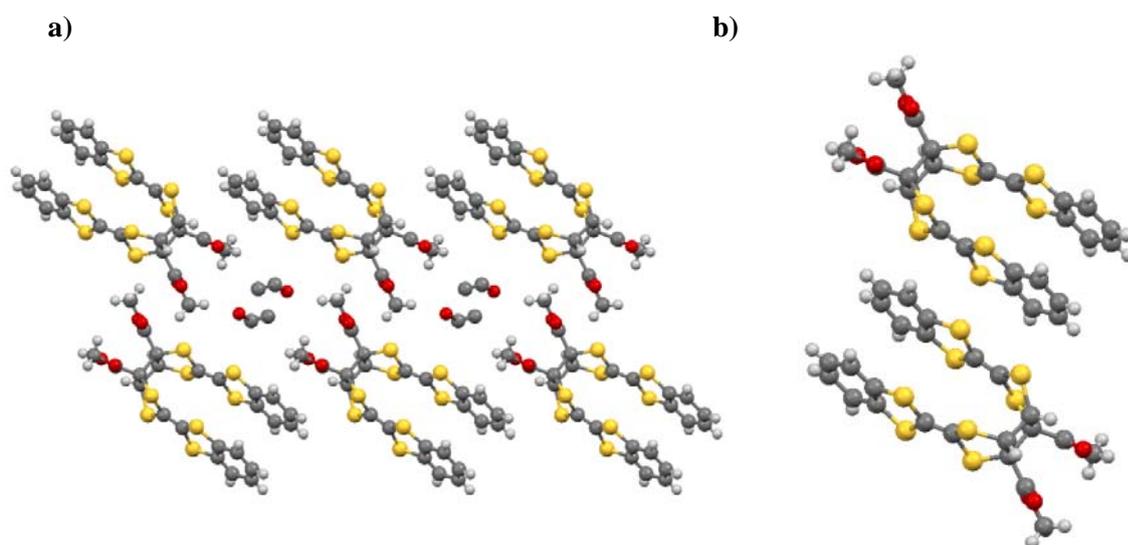


Figure S1. (a) Molecular diagram and (b) crystal packing of **3** in the *ac* plane, showing the intermolecular hydrogen bonding system.



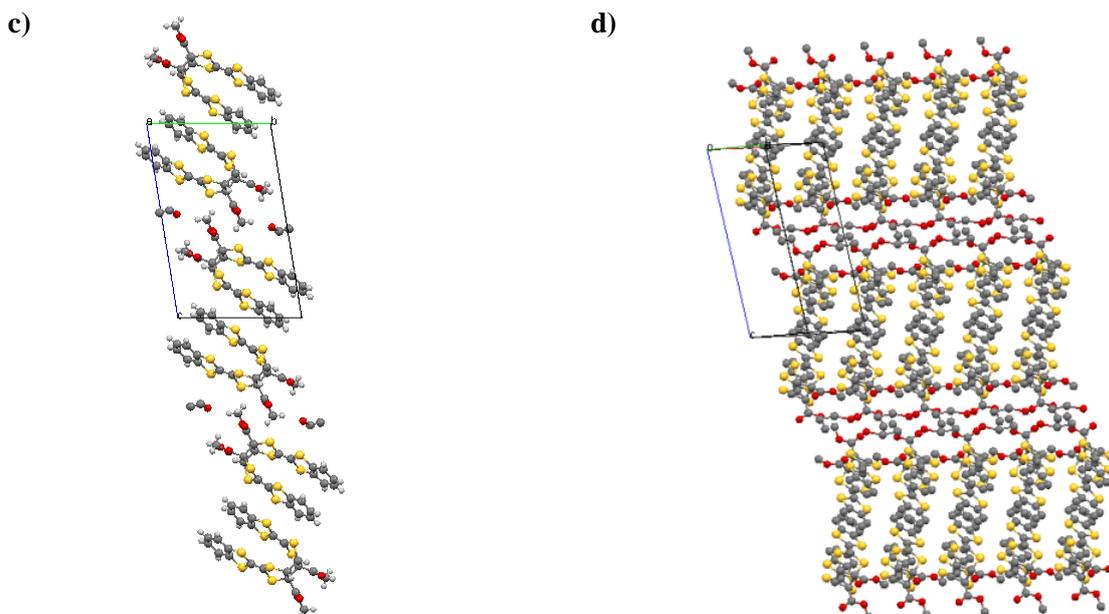


Figure S2. Crystal packing of **2** (a) in a view along the *a* axis, showing the ethanol molecules lying in the space left by the TTFH molecules, without establishing intermolecular interactions amongst them, the only classical hydrogen bonds being the ones established between ethanol...ethanol molecules; (b) detail of the packing showing the head-to-tail orientation along the *c* axis (c) showing the cisoid arrangement of the head-to-tail dimers along *a* and (d) the *ab* plane. A 2D sheet is formed showing the alternation of the layer of head to tail dimers and ethanol molecules.

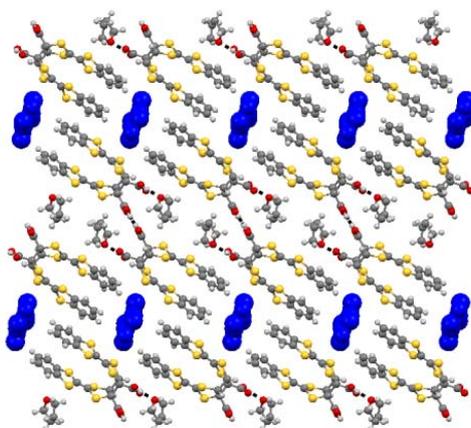


Figure S3. Crystal packing of **4** showing the disordered THF molecules (blue) lying in the space left between the hydrogen bonded groups.

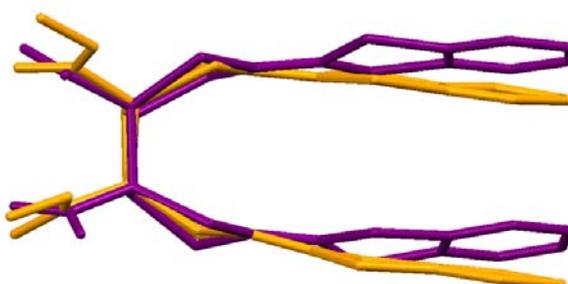


Figure S4. Overlap of the crystal structures of **2** (orange) and **4** (purple).

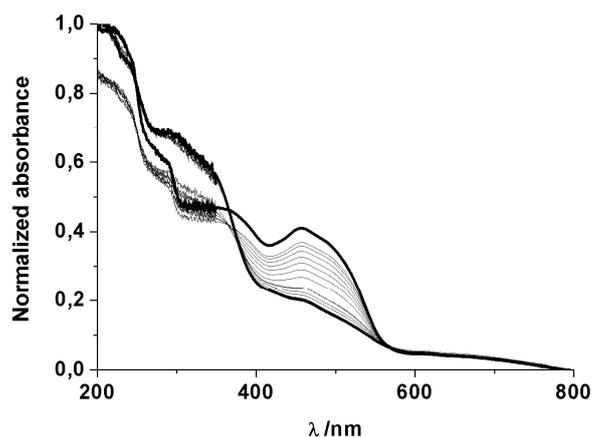


Figure S5. UV-Vis spectra of **1** drop-cast films recorded for different illumination time an HBO ((514 nm, 15 mW)) source. The arrows indicate the progression of bands along time. Bold lines correspond to the initial (0 min.) and final spectra (120 min).

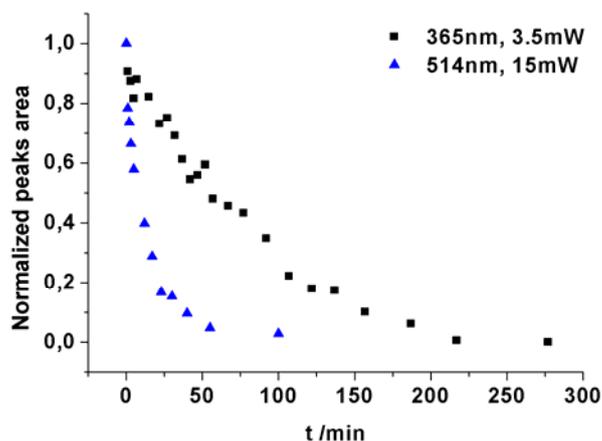


Figure S6. Kinetic rate dependence normalized to the intensity of the monomer **1** absorbance band at 450 nm, for HBO lamp (365 nm, 3,5 mW) and Ar ion laser (514 nm, 15 mW) irradiation sources.

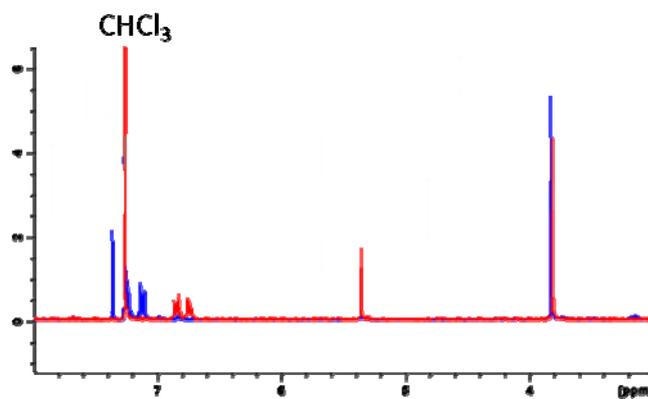


Figure S7. NMR spectrum of monomer **1** (blue) and dimer **2** (red) in CDCl_3 solution.