Supplementary information for the paper

The first tetrathiafulvalene–σ–polynitrofluorene diads: low HOMO – LUMO gap, amphoteric redox behavior and charge transfer properties

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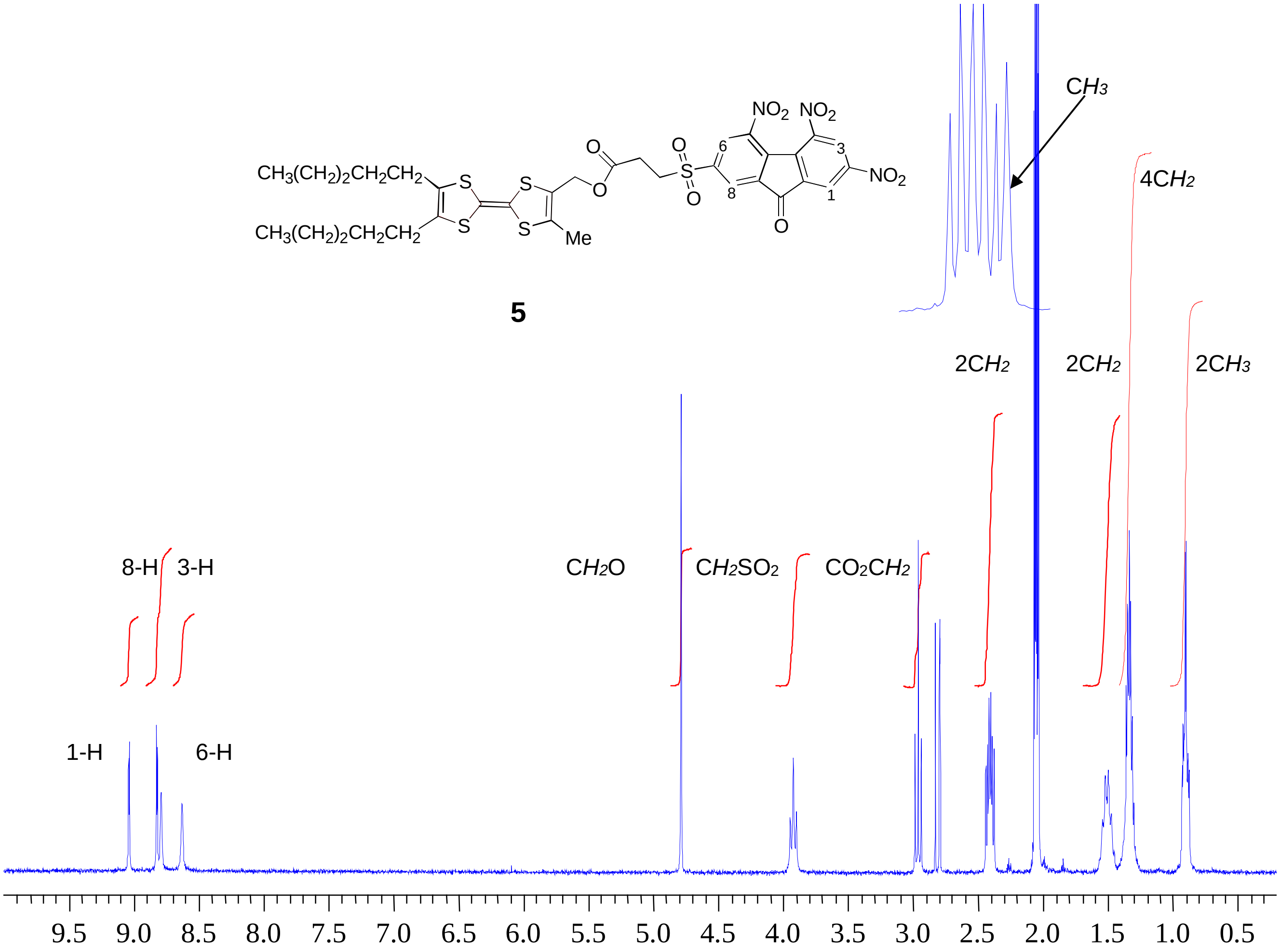

Figure S1. ^{1}H NMR spectra of compound **5** in acetone-d_6.

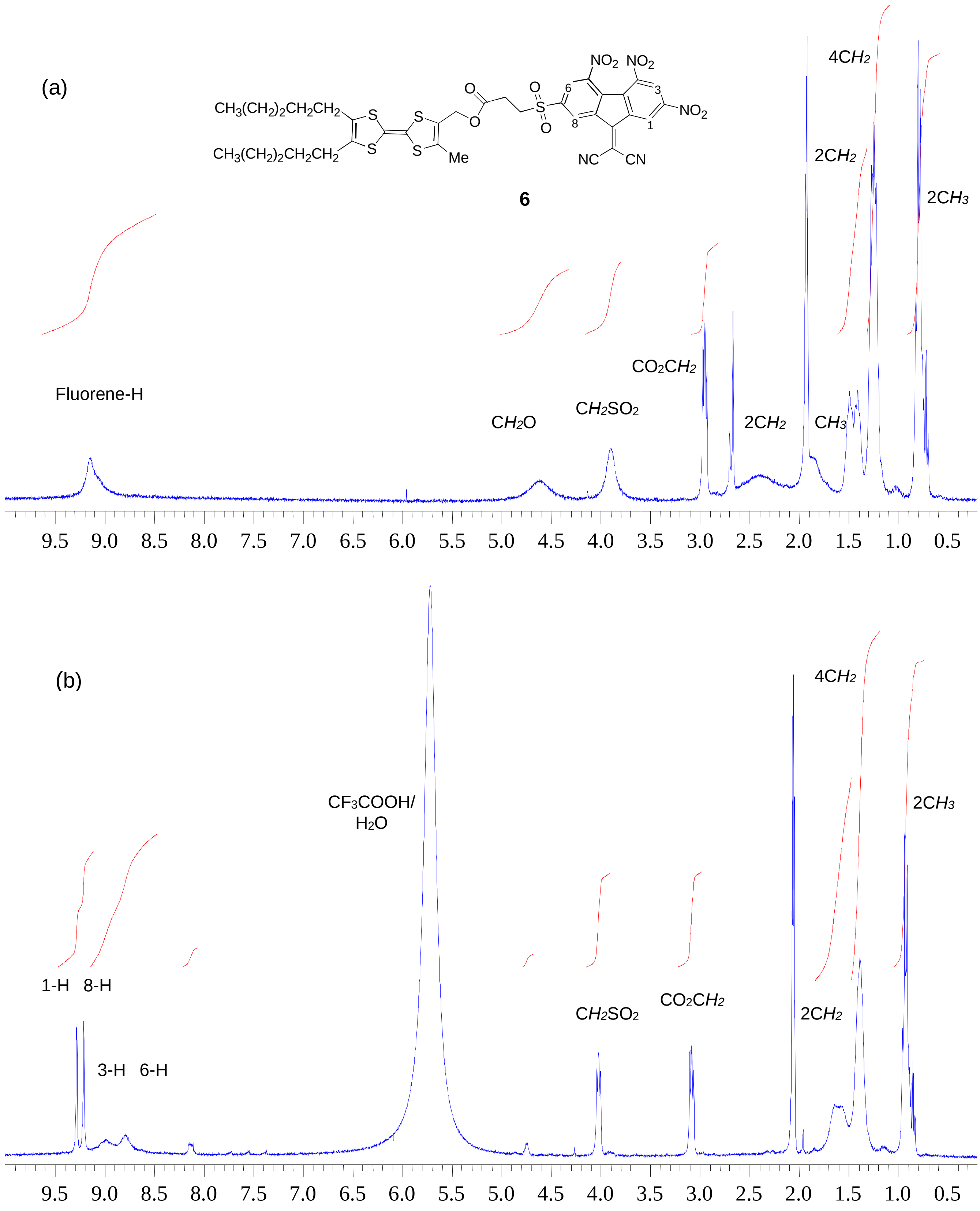

Fig. S2. ^{1}H NMR spectra of compound **6** in acetone-d_6 as prepared (a) and after adding a drop of CF_3COOH (b).

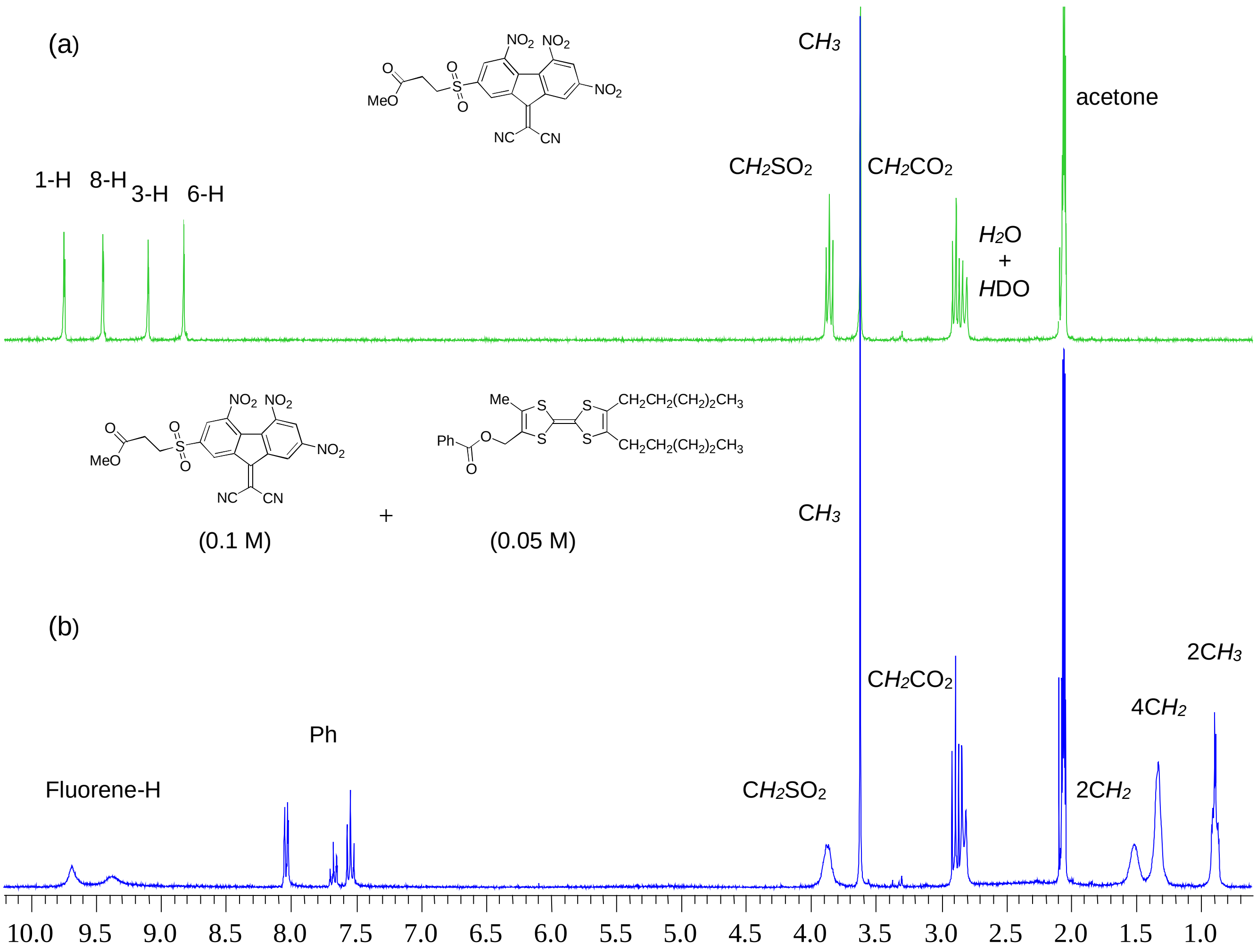

Fig. S3. Paramagnetic broadening in ^{1}H NMR spectra of acceptor **7** (a)[1] after adding donor **2a** (b)[2], in acetone-d_6.

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[1] Fluorene protons give doublets (J = 2 Hz).

[2] Due to paramagnetic broadening, signals of protons, adjacent to TTF moiety are very broad and can not be seen on this graph (in pure compound **2a** all the protons give sharp NMR signals).

Semiempirical calculations.

The geometry of compound **6** was optimized using the MNDO-PM3 semiempirical method as implemented in the HyperChem 5.02 package of programs. Polak-Ribiere algorithm was used for the optimization with SCF convergence limit of 1×10^{-5}; the gradient norm achieved was less than 0.005 kcal mol^{-1} Å^{-1}. Due to flexibility of the σ-spacer a number of minima with close energy were found. Fig. S3 shows "head-to-tail" and "extended" conformations of the molecule.

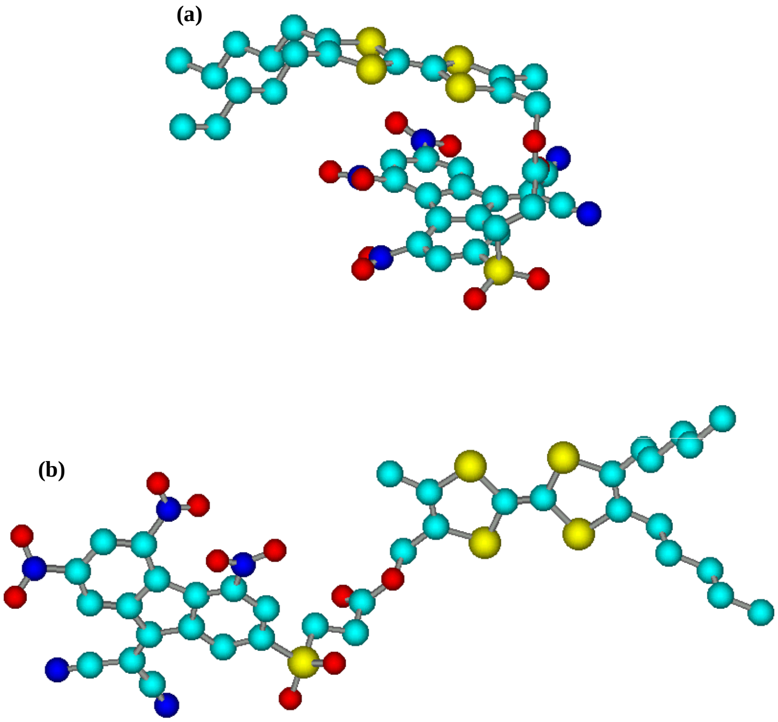

Figure S4. Optimized geometries of (a) a "head-to-tail" (heat of formation 22.96 kcal mol^{-1}) and (b) an "extended" (heat of formation 22.39 kcal mol^{-1}) conformations of **6**.