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Supplementary Information For:

Electrochromic tetrathiafulvalene derivatives functionalised with 2,5-diaryl-1,3,4-oxadiazole chromophores

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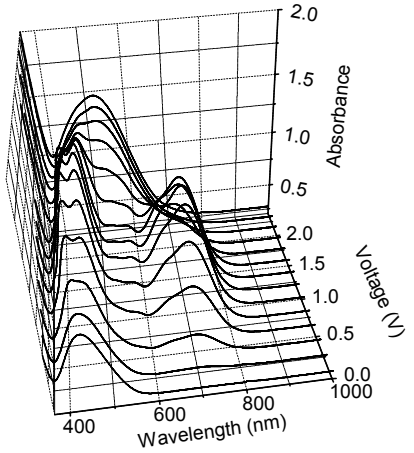
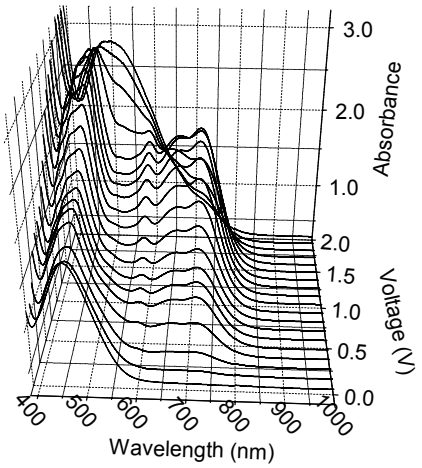
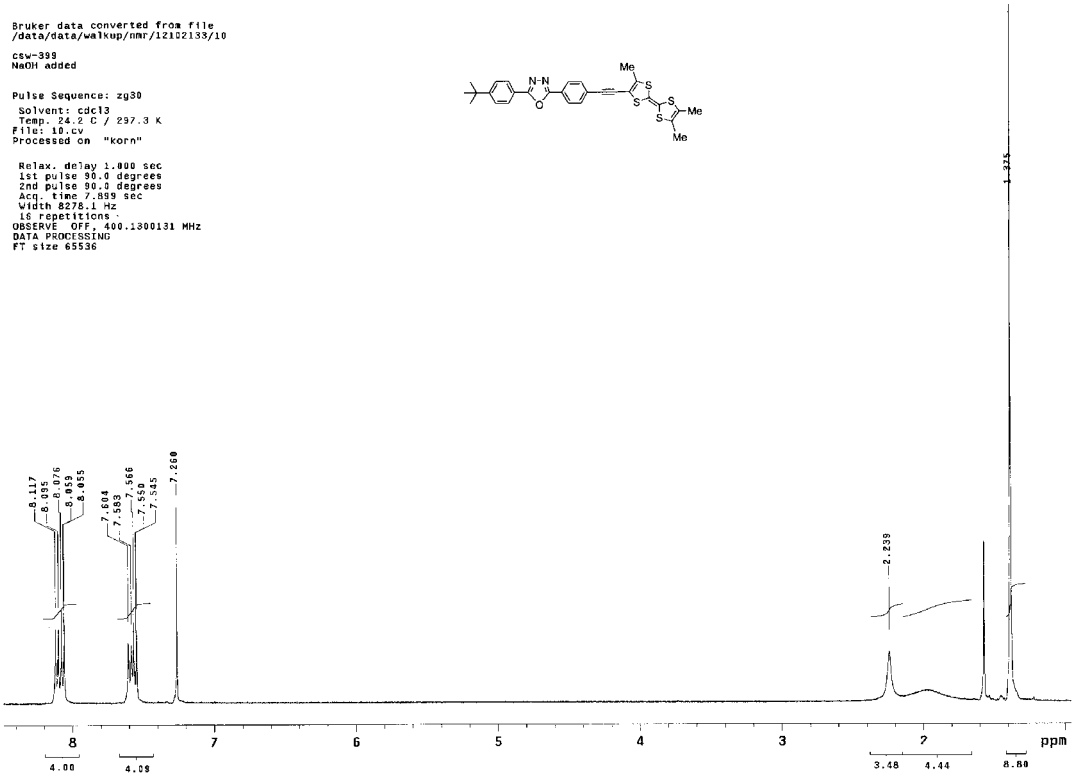
1. Absorption spectroelectrochemistry of **3**. Measured under the conditions in the caption to Fig 2.



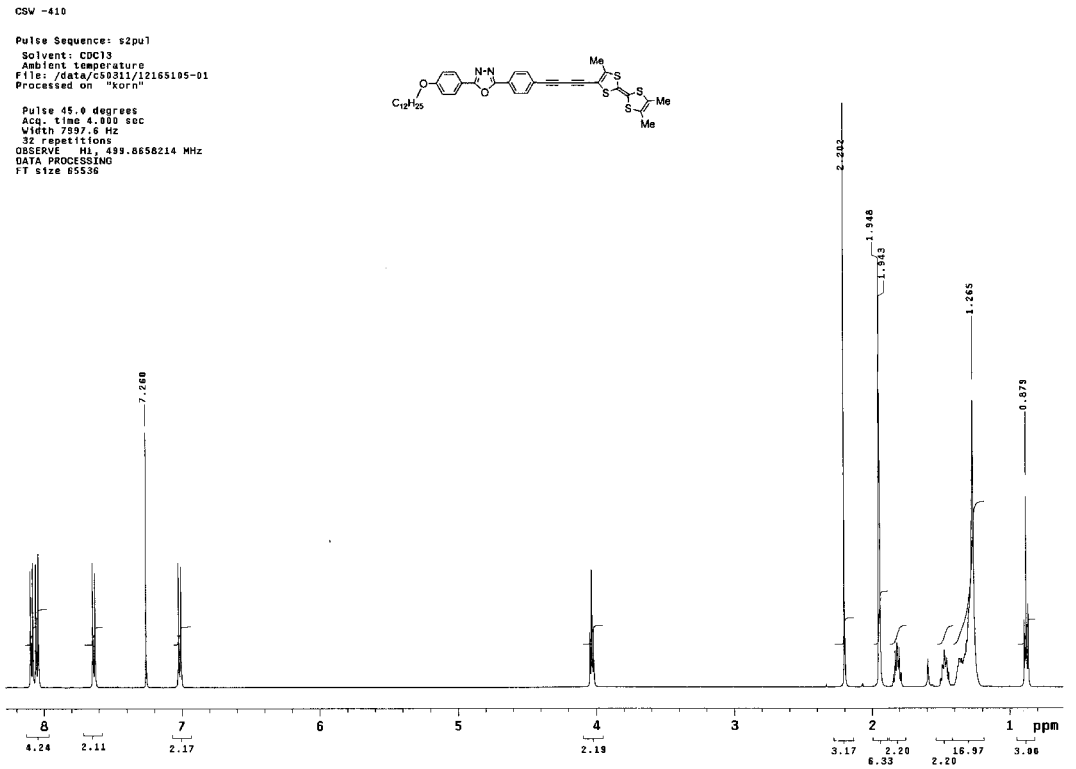
2. Absorption spectroelectrochemistry of **4**. Measured under the conditions in the caption to Fig 2.



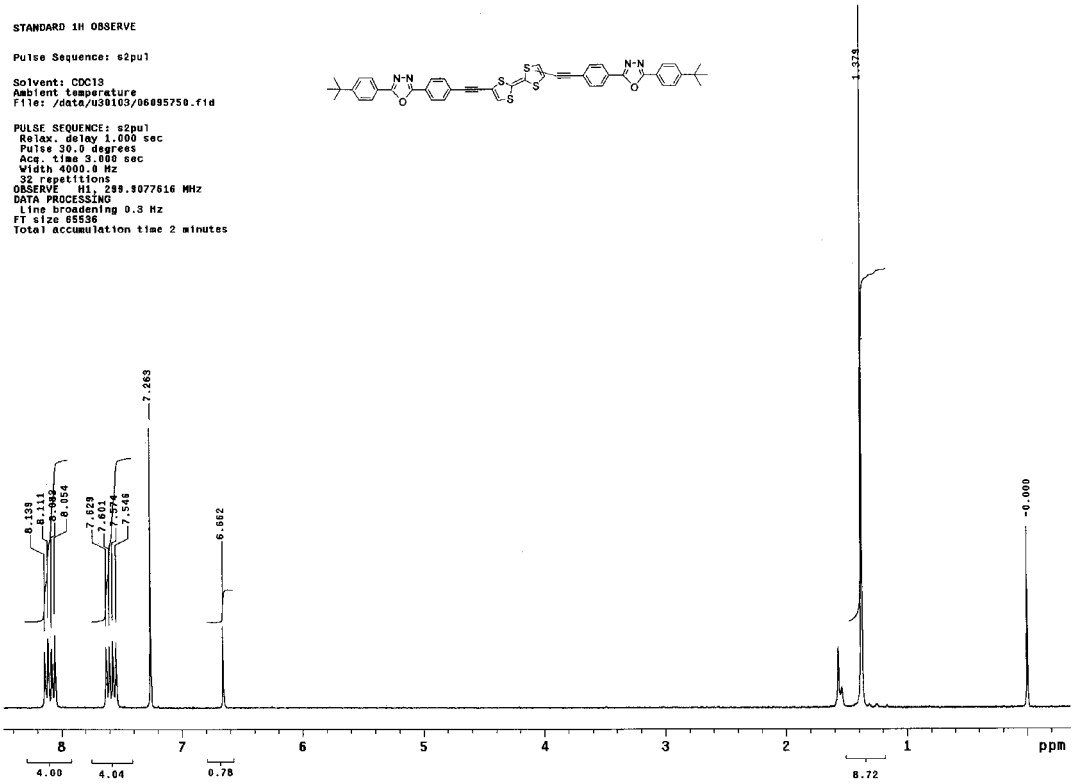
3. ^{1}H NMR of compound **3**, measured in $CDCl_3$ treated with NaOH.



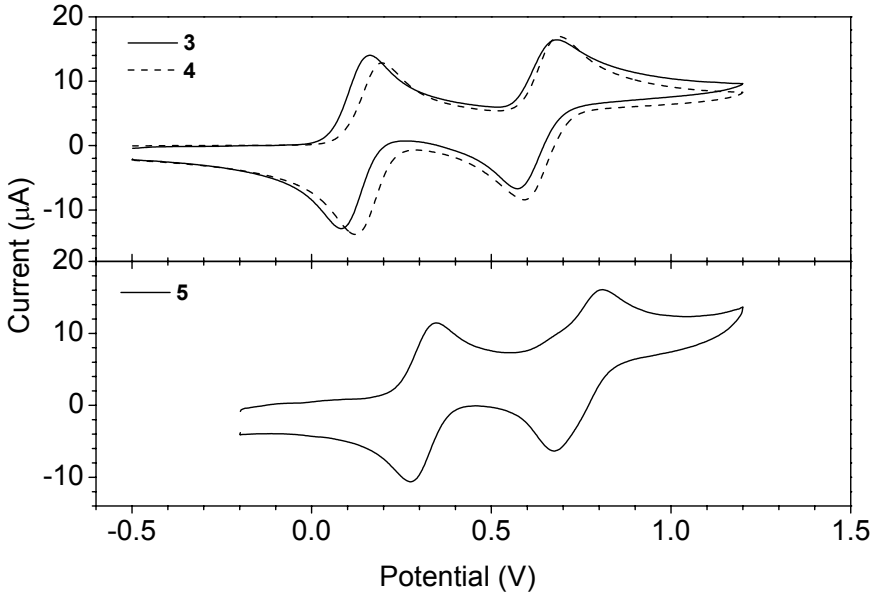
4. ^{1}H NMR of compound **4**, measured in $CDCl_3$ treated with NaOH.



5. ^{1}H NMR of compound **5**.



6. Cyclic voltammograms of compounds **3**-**5**. Supporting electrolyte: 0.1 M $TBAPF_6$ in DCM. Electrodes: working; Pt disk (Φ = 1.8 mm); counter, Pt wire; reference, $Ag/AgNO_3$ in acetonitrile. Scan rate: 100 mV/sec.



7. Further crystallographic information for compound **5**.

The structure was solved by direct methods and refined by full-matrix least squares against F^2 of all reflections, using SHELX-97 software (G. M. Sheldrick, Göttingen University, 1997).

Figure 1 was plotted at 50% displacement ellipsoids. One *t*-Bu group is disordered between two orientations with occupancies 60% (solid) and 40% (dashed, H atoms omitted), the likely disorder of the other *t*-Bu was not resolved. Molecule **5** has no crystallographic symmetry, and the conformations of its two halves are rather dissimilar. The TTF moiety adopts an asymmetric boat conformation, folding along the S(1)···S(2) and S(3)···S(4) vectors by 11.6 and 5.3º, the outer S_2C_2 fragments *i* and *ii* are planar. The C(7) ≡ C(8) bond is tilted out of plane *i* by 10.2º, while the C(27) ≡ C(28) bond by only 1.5º from plane *ii*. The dihedral angles involving benzene (*iii*, *v*, *vi*, *viii*) and oxadiazole (*iv*, *vii*) rings are: *i*/*iii* 17.3, *iii*/*iv* 14.3, *iv*/*v* 20.0, *ii*/*vi* 38.5, *vi*/*vii* 21.7, *vii*/*viii* 16.2º. Nevertheless, the deviation of *all* non-hydrogen atoms (except methyl carbons) from their mean plane (average 0.19 Å, maximum 0.64 Å) is small compared to the overall length of the molecule (*ca*. 43 Å for the van der Waals' shape).

The structure being triclinic, long axes of all the molecules in the crystal are parallel to each other. Molecules form a loose stack (parallel to the *y* axis) with a mean "interplanar" separation of *ca*. 3.6 Å, as their puckering prevents closer approach. Molecules related by the *a* translation (and belonging to adjacent stacks) are linked into infinite chains by intermolecular contacts S(1)···S(2′) 3.57 and S(3)···S(4′) 3.60 Å (and their equivalents), which are comparable with the standard van der Waals' contact of 3.60 Å.[s1]

[S1] R. S. Rowland and R. Taylor, *J. Phys. Chem*., 1996, **100**, 7384.