Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Electronic Supplementary Information

Efficient synthesis of 3,4-alkoxythieno[2,3-b]thiophene derivatives. The first block copolymer associating 3,4-ethylenedioxythieno[2,3-b]thiophene (EDOThT) and 3,4-ethylenedioxythiophene (EDOT) moieties.

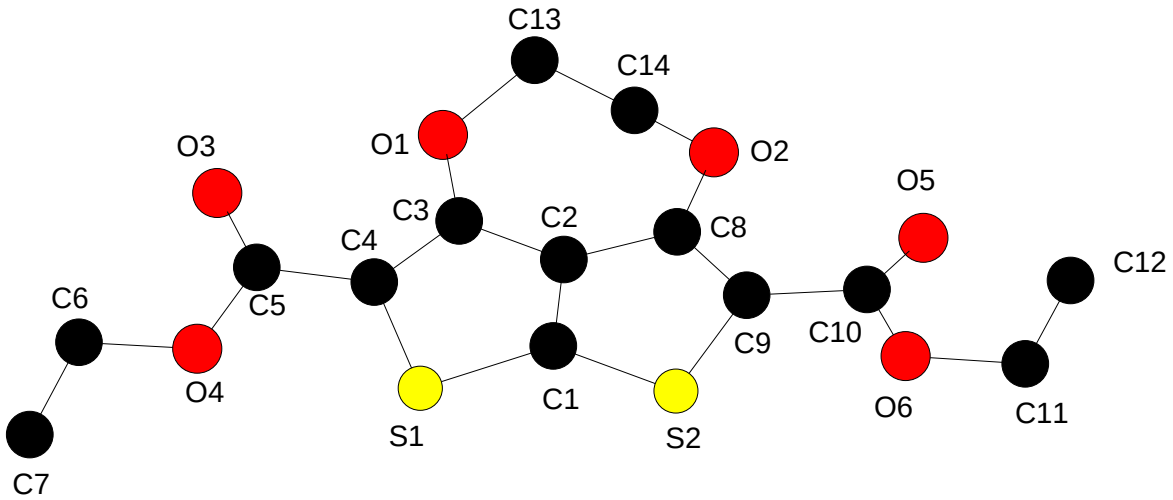
Noémie Hergué and Pierre Frère

Table of contents

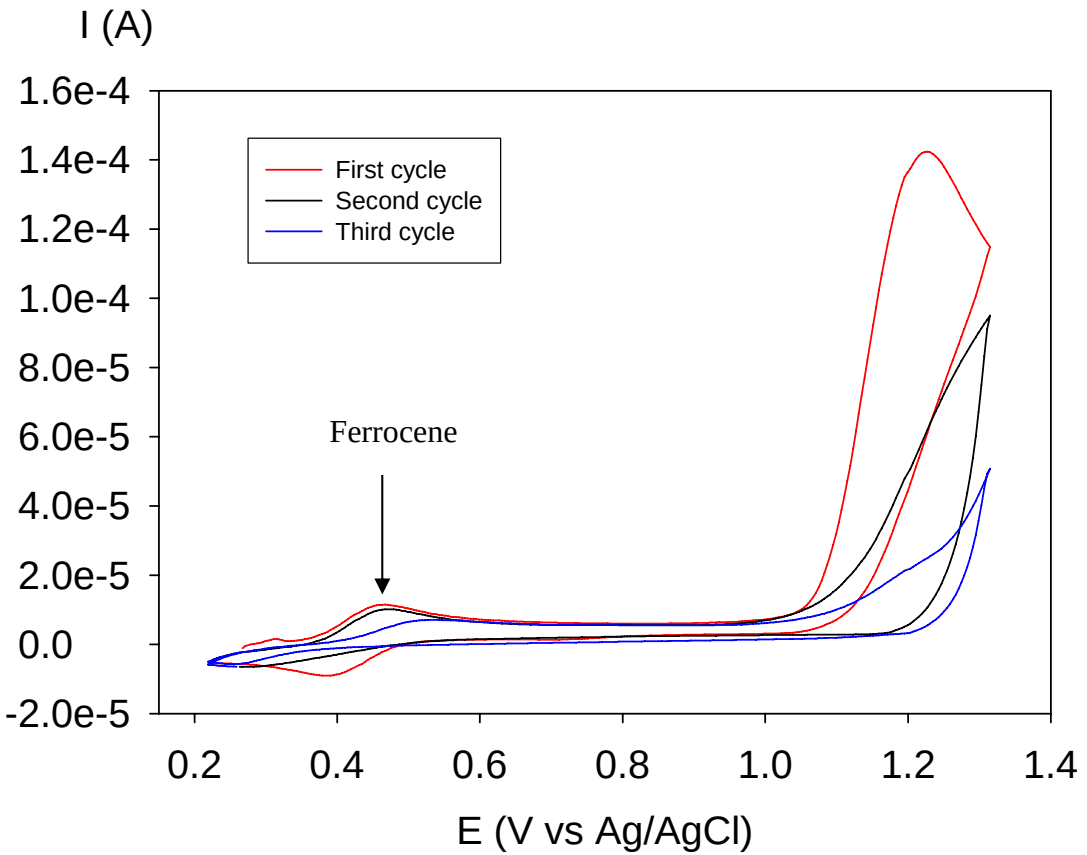
Crystal data and structure refinement for 2c.

Identification code	2c
Empirical formula	C14 H14 O6 S2
Formula weight	342.37
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 5.098(1) A alpha = 90 deg. b = 14.076(2) A beta = 92.82(2) deg. c = 20.831(7) A gamma = 90 deg.
Volume	1493.0(6) A^3
Z, Calculated density	4, 1.523 Mg/m^3
Absorption coefficient	0.383 mm^-1
F(000)	712
Crystal size	0.44 x 0.07 x 0.01 mm
Theta range for data collection	3.27 to 26.01 deg.
Limiting indices	-6<=h<=6, -17<=k<=16, -25<=l<=23
Reflections collected / unique	23632 / 2905 [R(int) = 0.1745]
Completeness to theta = 26.01	98.6 %
Absorption correction	Gaussian

Max. and min. transmission	0.9962 and 0.9260
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2905 / 0 / 201
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0851, wR2 = 0.1403
R indices (all data)	R1 = 0.1865, wR2 = 0.1718
Largest diff. peak and hole	0.491 and -0.415 e.A^-3



Electrooxidation of EDOThT



Electropolymerization of **EDOThT** at 10^{-2}M mol L^{-1} in 0.1M Bu_4NPF_6 in CH_2Cl_2, reference Ag/AgCl, v = 100 $mV.s^{-1}$ in presence of ferrocene (10^{-3} M).

Recurrent scans of EDOThT in presence of a small amount of ferrocene, the reversible oxidation peak of this latter vanished after three scans thus shown on the figure.