Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Bis - EDOT end capped by n-hexyl or n-hexylsulfanyl groups: Effect of the substituents on the stability of the oxidized states

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Supplementary information

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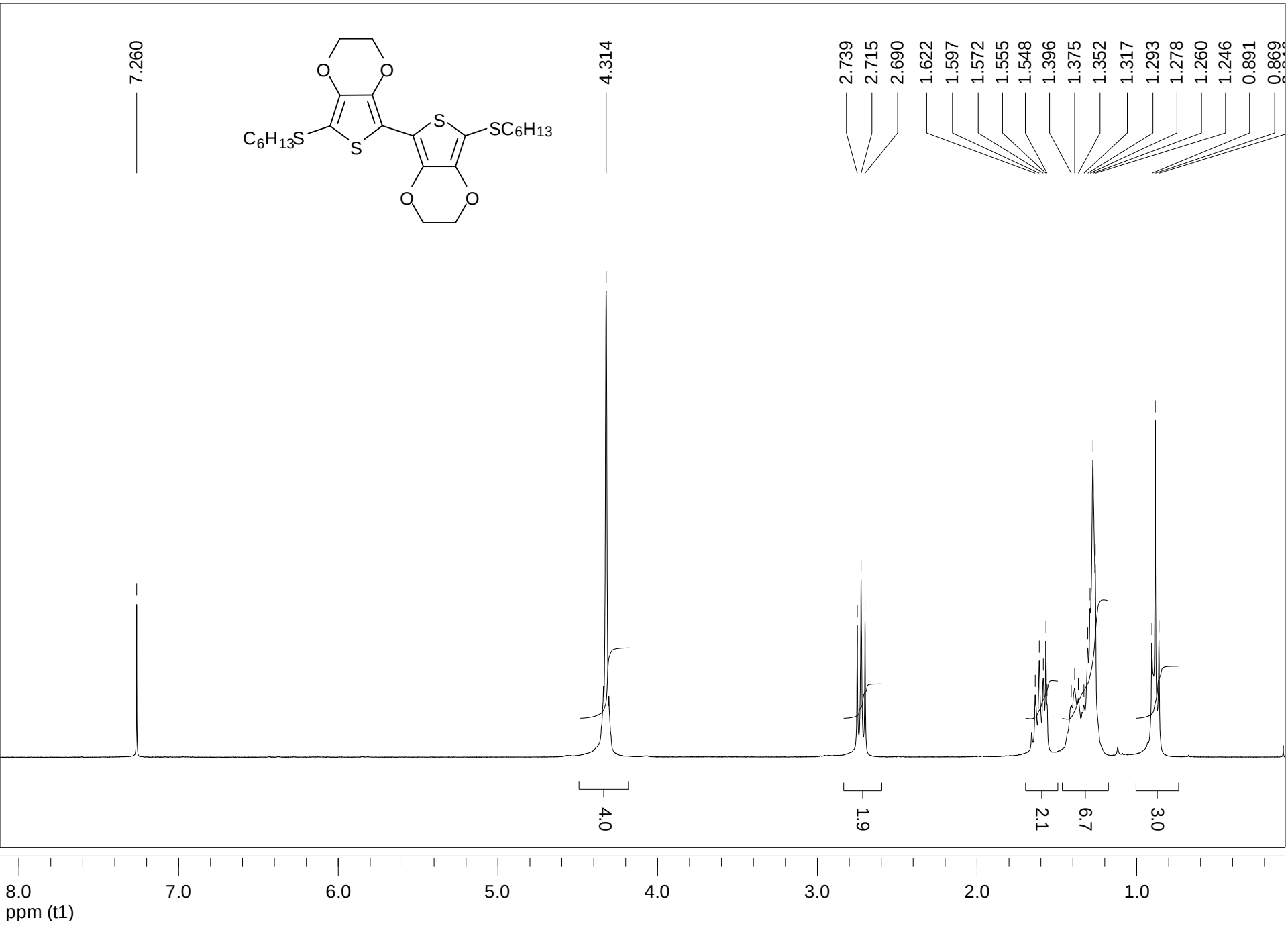
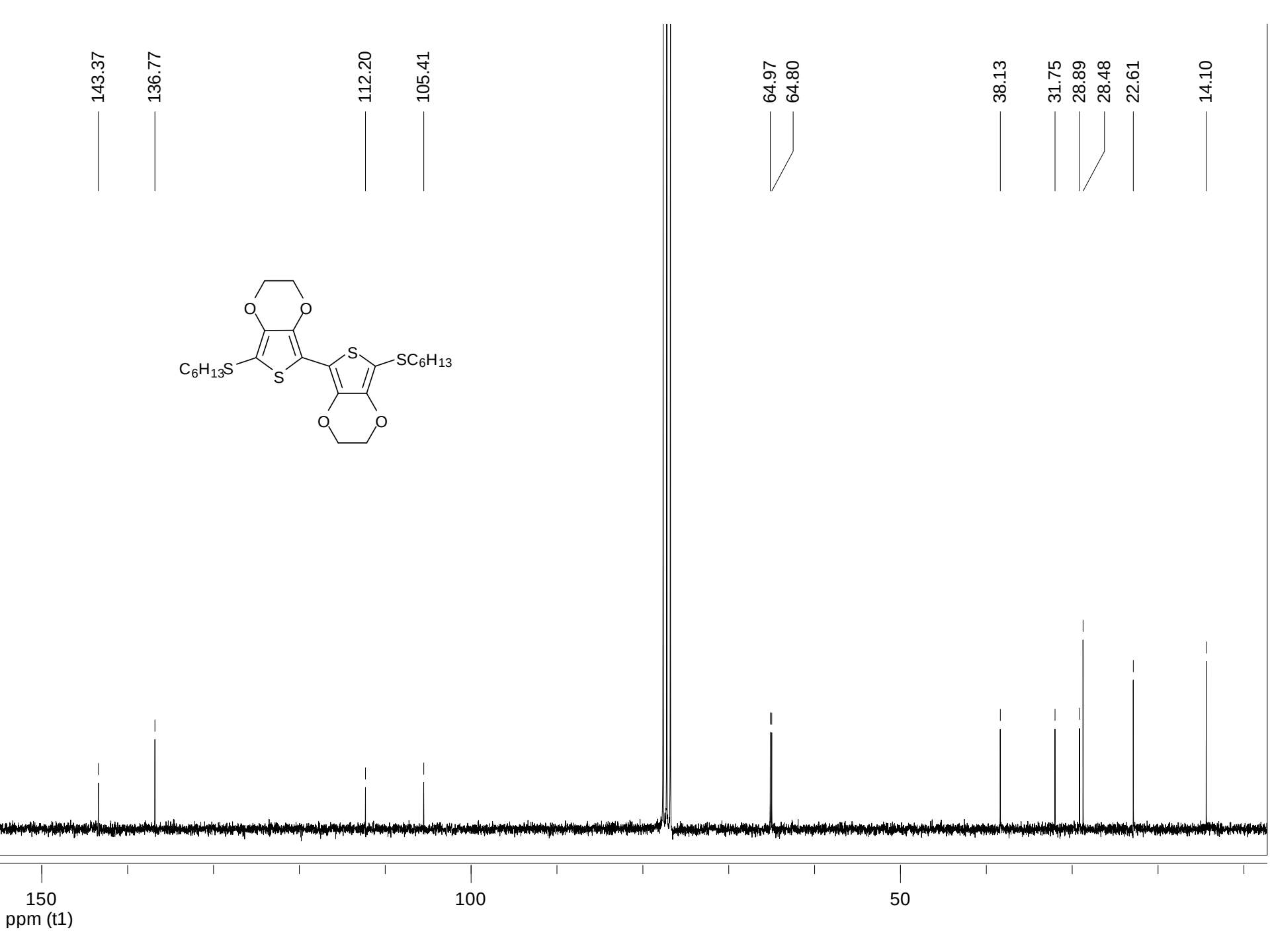
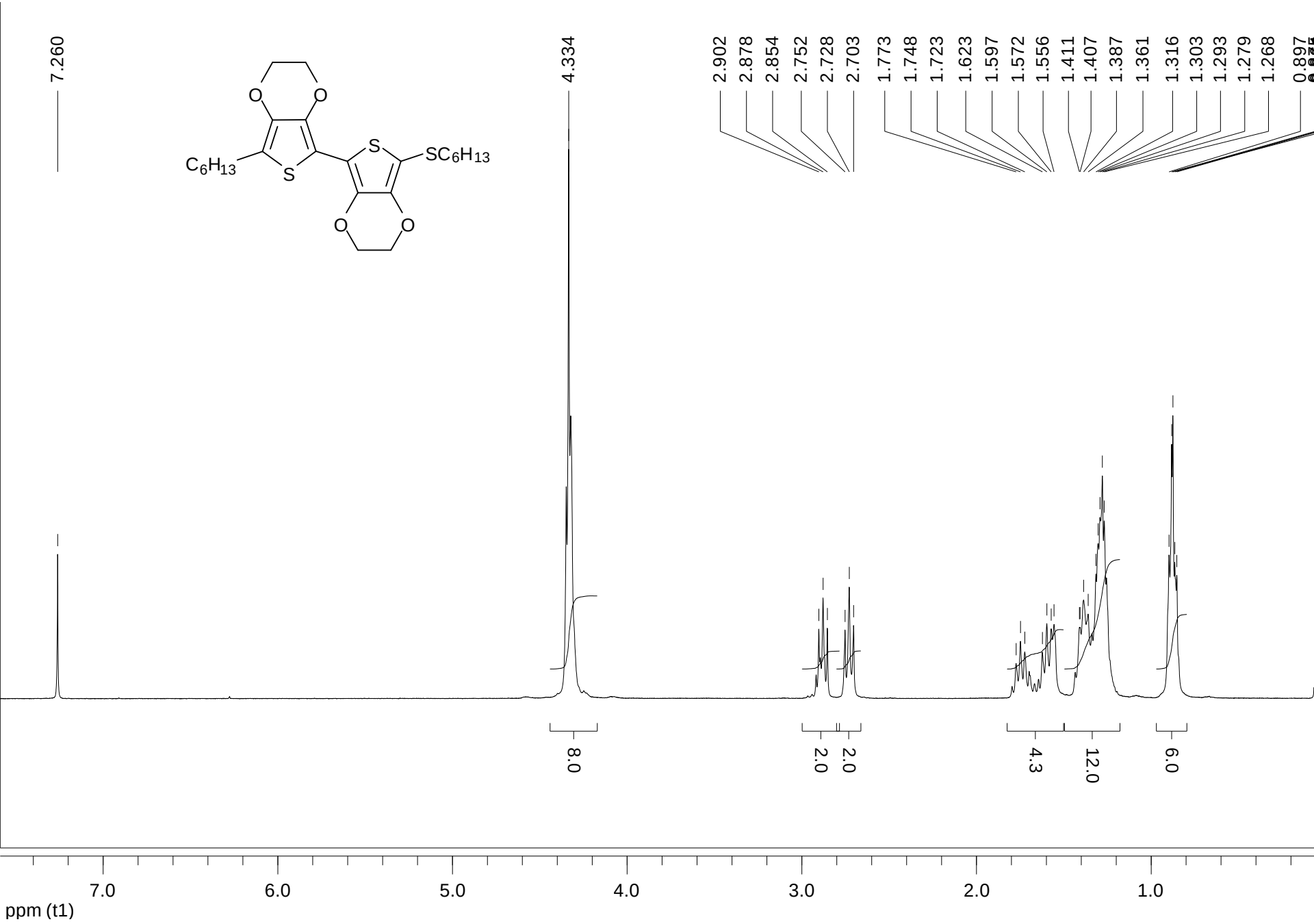
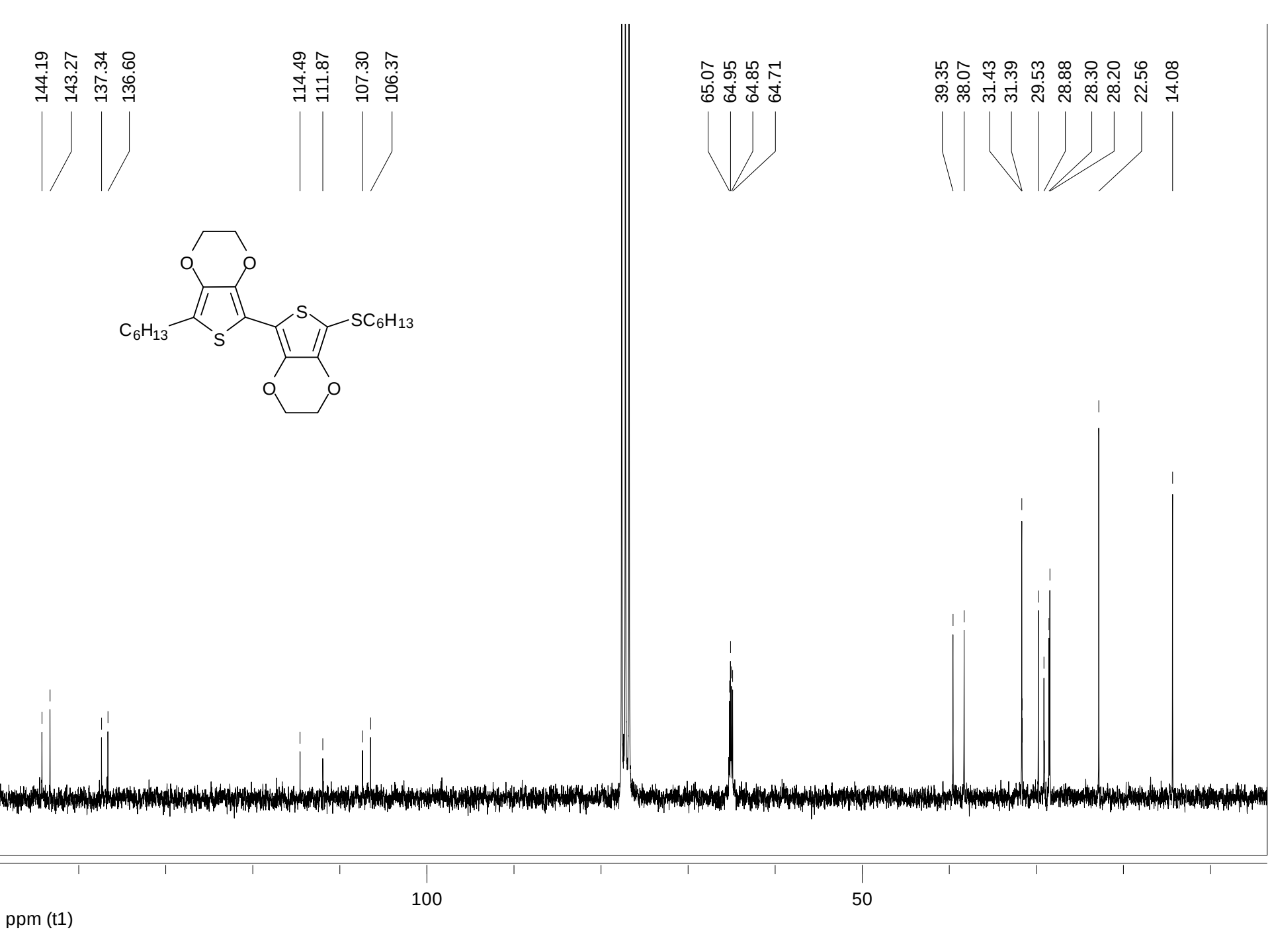

7.260
4.314
2.739
2.715
2.690
1.622
1.597
1.572
1.555
1.548
1.396
1.375
1.352
1.317
1.293
1.278
1.260
1.246
0.891
0.869
C6H13S
SC6H13
O
O
S
S
O
O
4.0
1.9
2.1
6.7
3.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


143.37
136.77
112.20
105.41
64.97
64.80
38.13
31.75
28.89
28.48
22.61
14.10
O
O
O
O
S
S
$C_6H_{13}S$
SC_6H_{13}
150
100
50
ppm (t1)


7.260
4.334
2.902
2.878
2.854
2.752
2.728
2.703
1.773
1.748
1.723
1.623
1.597
1.572
1.556
1.411
1.407
1.387
1.361
1.316
1.303
1.293
1.279
1.268
0.897
O
O
S
S
O
O
C6H13
SC6H13
8.0
2.0
2.0
4.3
12.0
6.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)


144.19
143.27
137.34
136.60
114.49
111.87
107.30
106.37
65.07
64.95
64.85
64.71
39.35
38.07
31.43
31.39
29.53
28.88
28.30
28.20
22.56
14.08
O
O
S
S
O
O
C6H13
SC6H13
100
50
ppm (t1)

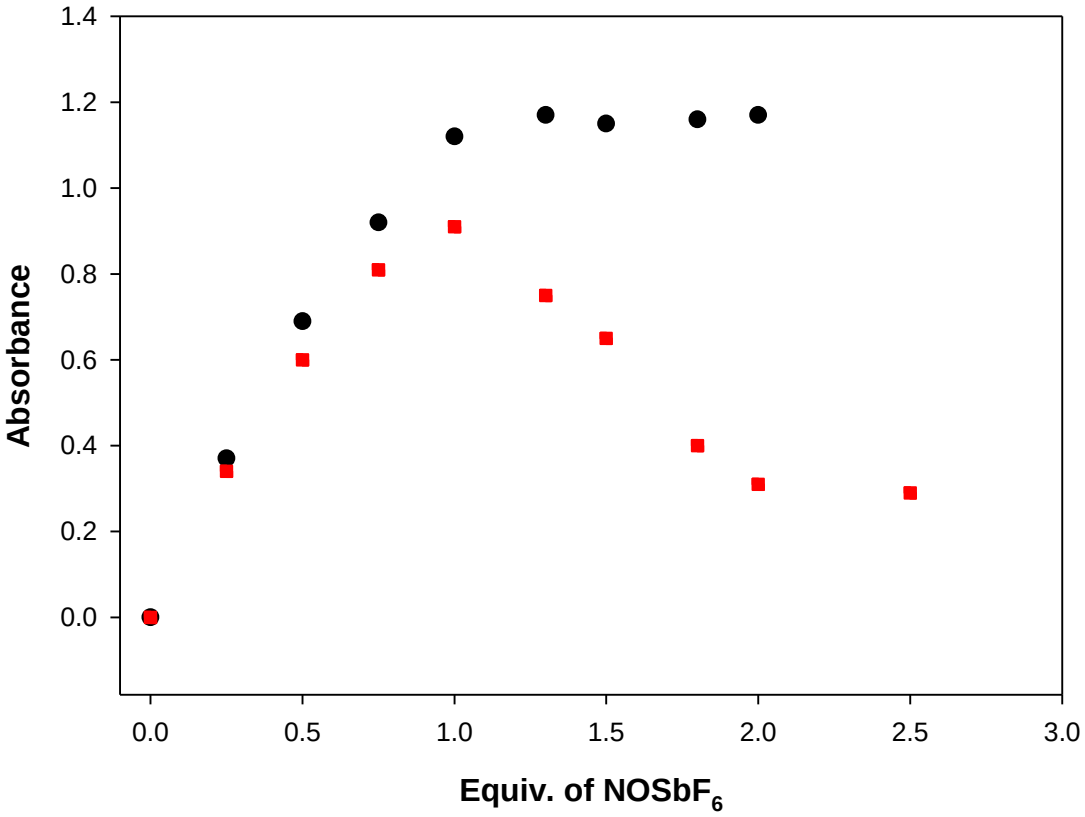
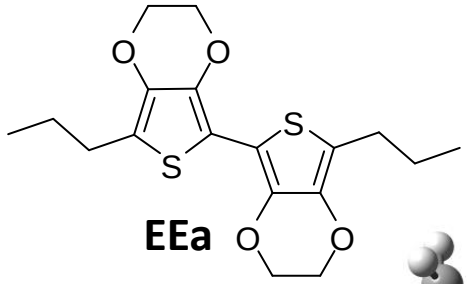
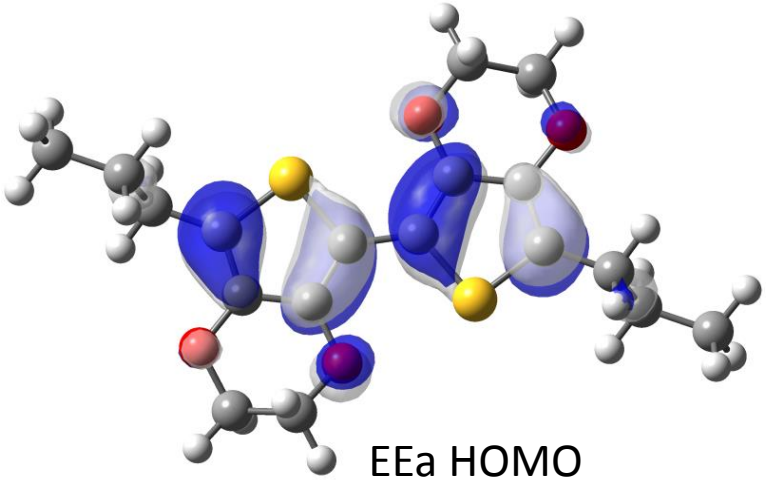


Figure S1 : Evolution of absorbance at λ = 440 nm (A_{440} black circle) for **EEa** 10^{-4} M in CH_2Cl_2 and at λ = 510 nm (A_{510} red square) for **EEb** 10^{-4} M in CH_2Cl_2 during the stepwise addition of $NOSbF_6$

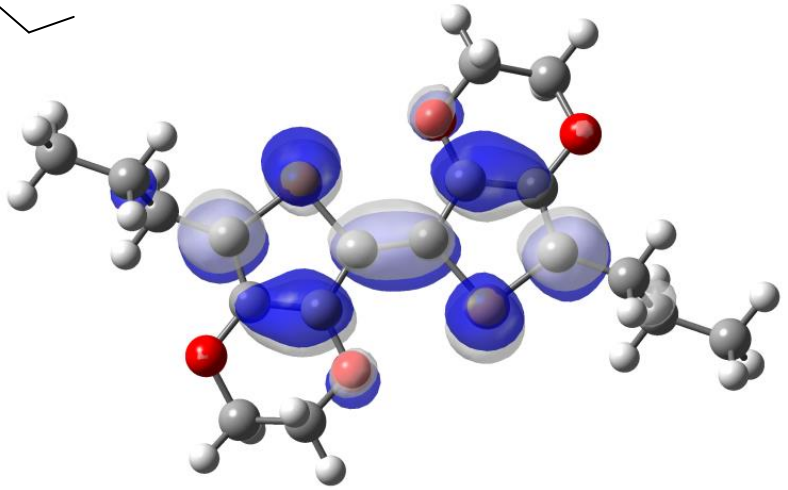
$NOSbF_6$ (10^{-2} M in CH_3CN) was added with a microsyringe to 5mL of **EEa** or **EEb** solution 10^{-4} M in CH_2Cl_2.
1 equivalent of $NOSbF_6$ corresponds to 50 µL of oxidant solution.



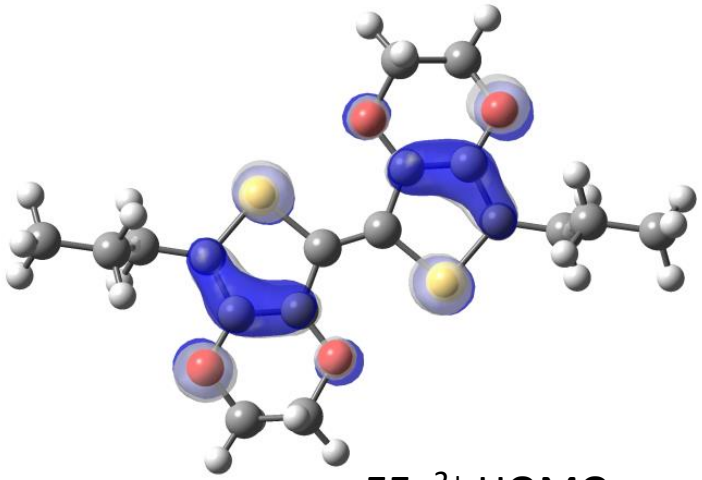
EEa



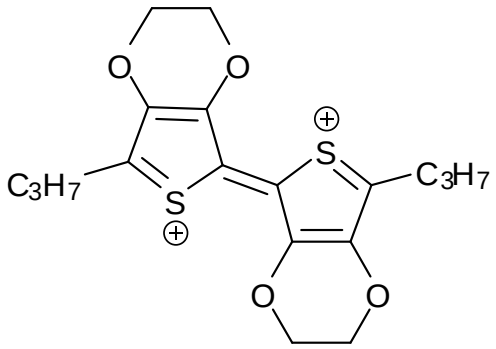
EEa HOMO



EEa LUMO

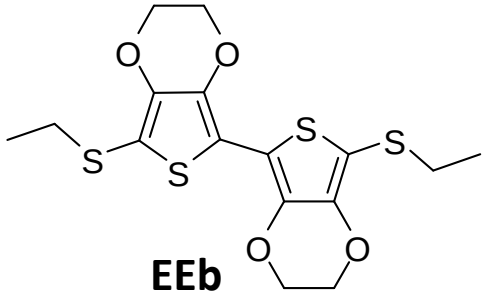


EEa^{2+} HOMO

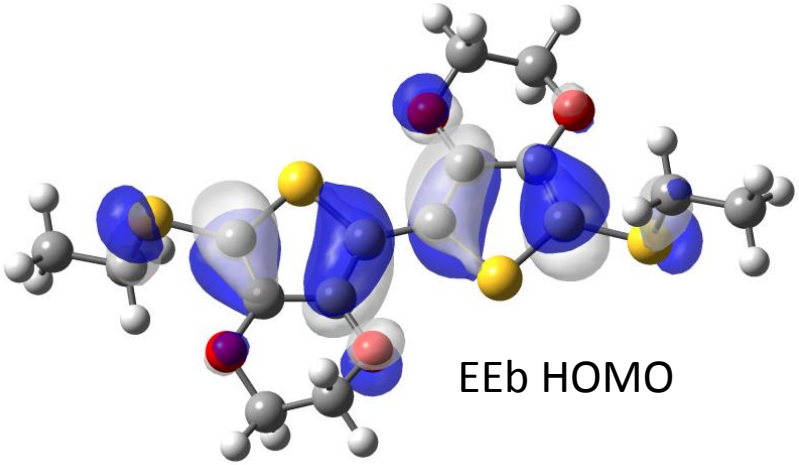


EEa^{2+}

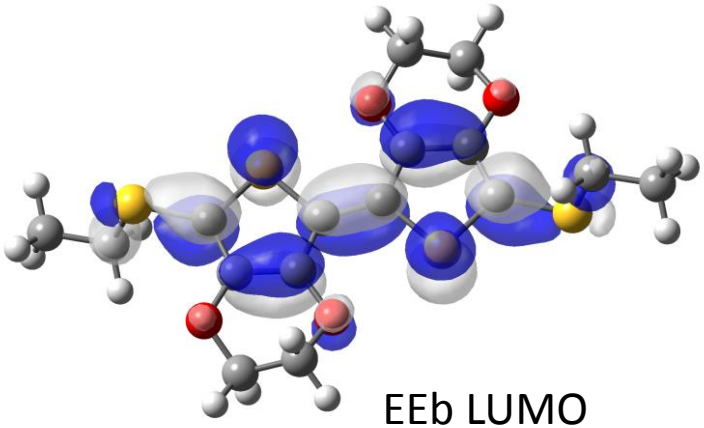
Gaussian09 B3LYP 6,31g (d,p)



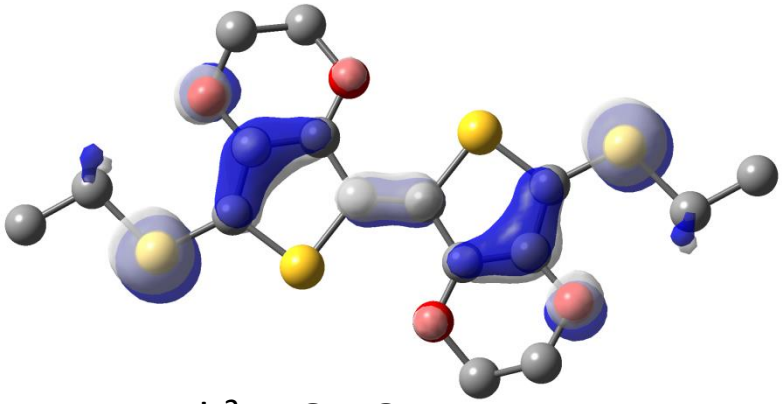
EEb



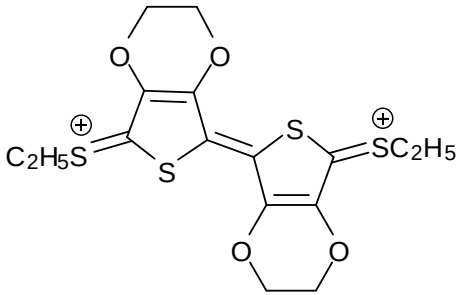
EEb HOMO



EEb LUMO

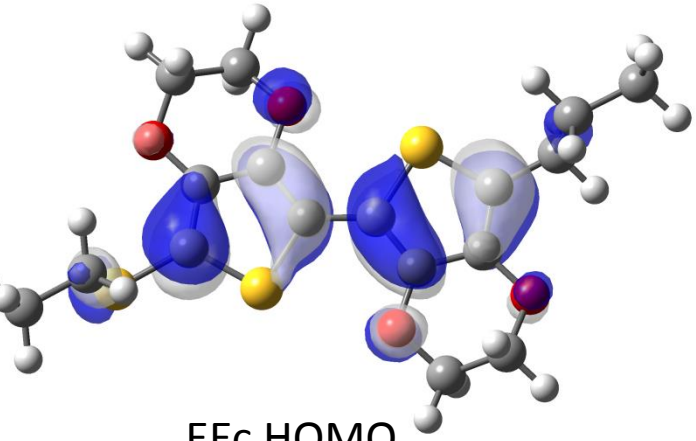


EEb^{2+} HOMO

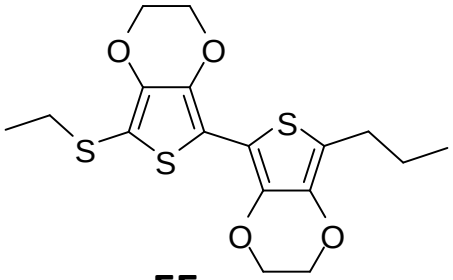


EEb^{2+}

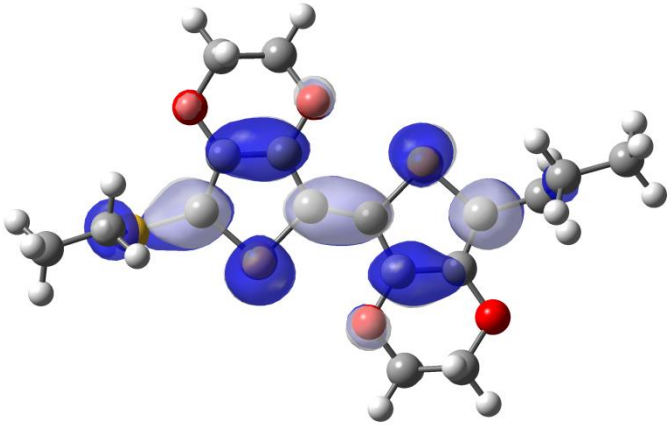
Gaussian09 B3LYP 6,31g (d,p)



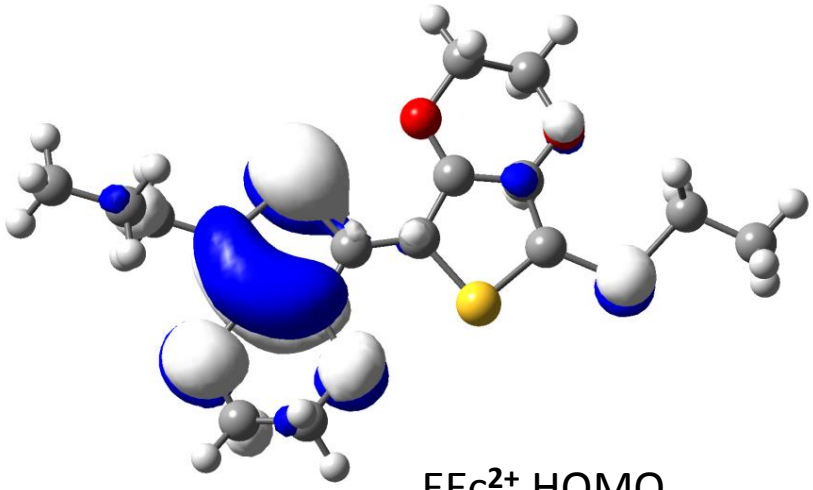
EEc HOMO



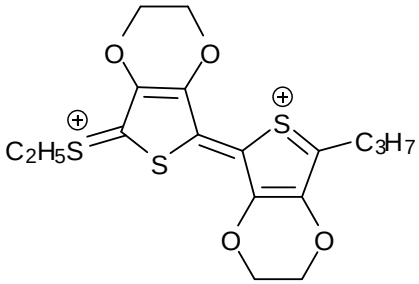
EEc



EEc LUMO



EEc^{2+} HOMO



EEc^{2+}

Gaussian09 B3LYP 6,31g (d,p)