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Solution-phase microwave-assisted synthesis of unsubstituted and modified α -quinque and sexithiophenes

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SUPPORTING INFORMATION

Contents:

- Optical micrographs under polarized and unpolarized light of a melted drop of compound **9** (T6) prepared according to the modalities described in Scheme 2 (page S2)
- First heating and cooling DSC plots of compound **11** prepared according to the modalities described in Scheme 3 (page S3)
- First heating DSC plot of compound **13** prepared according to the modalities described in Scheme 3 (page S3)
- First cooling DSC plot of compound **13** prepared according to the modalities described in Scheme 3 (page S5)
- Optical micrographs under polarized (left) and unpolarized (right) light of a melted drop of compound **13** (page S6)
- ¹H NMR spectrum of compound **10** in CDCl₃ (page S7)
- ¹³C NMR spectrum (APT) of compound **10** in CDCl₃ (page S8)
- Normalized absorption and photoluminescence spectra of compounds **24** and **25** in methylene chloride (page S9)
- Optimized cartesian coordinates of compounds **24** and **25** (pages S10-S13)

General details. PdCl₂(dppf), KF, *n*-BuLi, Pd(PPh₃)₂Cl₂, PPh₃, CuI, diisopropylamine, 2-bromo-4-methyl-thiophene, α -bithiophene (**1**), 2-thiophene boronic acid (**3**), α -terthiophene (**4**), bis(pinacolato)diboron (**8**), 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane and 5-formyl-2-thiophene boronic acid (**14**) are commercially available compounds. Flash chromatographies were carried out using silica gel (200-300 mesh ASTM). Analytical thin layer chromatographies (TLC) were carried out using 0.2 mm sheets of silica gel 60 F₂₅₄ and the visualization accomplished by UV lights (356 nm and 254 nm). Microwave assisted reactions were carried out in air using a commercial system Synthwave 402, with variable power and fixed temperature.

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Optical micrographs under polarized (left) and unpolarized (right) light of a melted drop of compound **9** (T6) prepared according to the modalities described in Scheme 2 (page S2)

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Normalized absorption and photoluminescence spectra of TATTAT (**24**, left) and TATTAT (**25**, right) in methylene chloride.

Compound 24 (TATTAT)

1	C	0.033378	-0.250198	-0.009961
2	C	0.020365	-0.250963	1.452044
3	C	1.066798	-0.403259	2.297213
4	C	0.691665	-0.359795	3.672936
5	C	-0.636567	-0.176124	3.852374
6	S	-1.462318	-0.034719	2.329988
7	C	-0.953065	-0.631741	-0.854876
8	C	-0.596800	-0.507366	-2.230679
9	C	0.657559	-0.033651	-2.410430
10	S	1.431195	0.288861	-0.888263
11	H	2.075196	-0.562756	1.965682
12	H	1.382250	-0.469387	4.486338
13	C	-1.346883	-0.092801	5.082860
14	H	-1.900949	-1.010755	-0.523090
15	H	-1.245759	-0.768241	-3.043905
16	C	1.331789	0.204112	-3.641068
17	C	1.911943	0.410484	-4.661362

18 C	2.586736	0.648509	-5.892814
19 C	-1.958478	-0.019400	6.103022
20 C	-2.669399	0.064051	7.334325
21 C	-3.989488	0.303383	7.511078
22 C	-4.371223	0.318979	8.889946
23 C	-3.332858	0.091909	9.716449
24 S	-1.859581	-0.148772	8.857593
25 H	-4.668355	0.463426	6.695972
26 H	-5.375067	0.493009	9.227093
27 H	-3.345268	0.051527	10.786615
28 C	3.820811	1.174676	-6.069922
29 C	4.189716	1.273315	-7.448843
30 C	3.227698	0.820767	-8.275033
31 S	1.844494	0.259895	-7.415804
32 H	3.248861	0.783185	-9.345163
33 H	5.129949	1.665456	-7.786251
34 H	4.447153	1.482118	-5.255033

Compound 25 (TATTTAT)

1 S	-7.373372	0.476965	7.159577
2 C	-7.273198	0.382937	8.876355
3 C	-6.000125	0.301257	9.306992
4 C	-5.054954	0.312653	8.232835
5 C	-5.642537	0.403174	7.017232
6 C	-5.004941	0.439818	5.744196
7 C	-4.489253	0.471768	4.670307
8 C	-3.852034	0.508434	3.398250
9 S	-2.119370	0.521762	3.264022
10 C	-2.206718	0.584040	1.530693
11 C	-3.493206	0.576943	1.109439
12 C	-4.436767	0.532961	2.178670
13 C	-0.990929	0.630931	0.720429
14 C	0.212229	1.156180	1.043481
15 C	1.178313	1.040285	-0.002440
16 C	0.698128	0.428328	-1.108229
17 S	-0.957203	-0.050667	-0.878511
18 C	1.391669	0.152413	-2.365105
19 C	0.863973	0.054250	-3.607869
20 C	1.837512	-0.219673	-4.614190

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21 C	3.092455	-0.324529	-4.120214
22 S	3.108804	-0.105297	-2.396267
23 C	4.293791	-0.581698	-4.838669
24 C	5.309767	-0.797343	-5.423034
25 C	6.512045	-1.054648	-6.141931
26 C	7.756053	-1.223843	-5.636998
27 C	8.737912	-1.466372	-6.649136
28 C	8.211812	-1.474343	-7.888486
29 S	6.513456	-1.188670	-7.875001
30 H	-8.164986	0.393332	9.469352
31 H	-5.723515	0.234431	10.341731
32 H	-3.991859	0.255612	8.364914
33 H	-5.500375	0.528597	2.039745
34 H	-3.775893	0.621823	0.074917
35 H	0.413705	1.639427	1.980652
36 H	2.176599	1.427949	0.072070
37 H	-0.179707	0.190366	-3.818504
38 H	1.608720	-0.324206	-5.656930
39 H	7.971281	-1.179149	-4.586975
40 H	9.778881	-1.624838	-6.441923
41 H	8.724122	-1.632372	-8.815635