Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Outside rules inside: the Role of the Electron-active Substituents in Thiophene-based Heterophenoquinones

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1. UV-Vis absorption and photoluminescence spectra of aromatic compounds

UV-vis absorption spectra were recorded on a Cary 5000 spectrophotometer (Varian), while photoluminescent spectra were recorded with a Jasco FP6600.
Photoluminescence spectra of the aromatic species were collected with very dilute solutions to avoid aggregation phenomena and minimize internal filter effects.

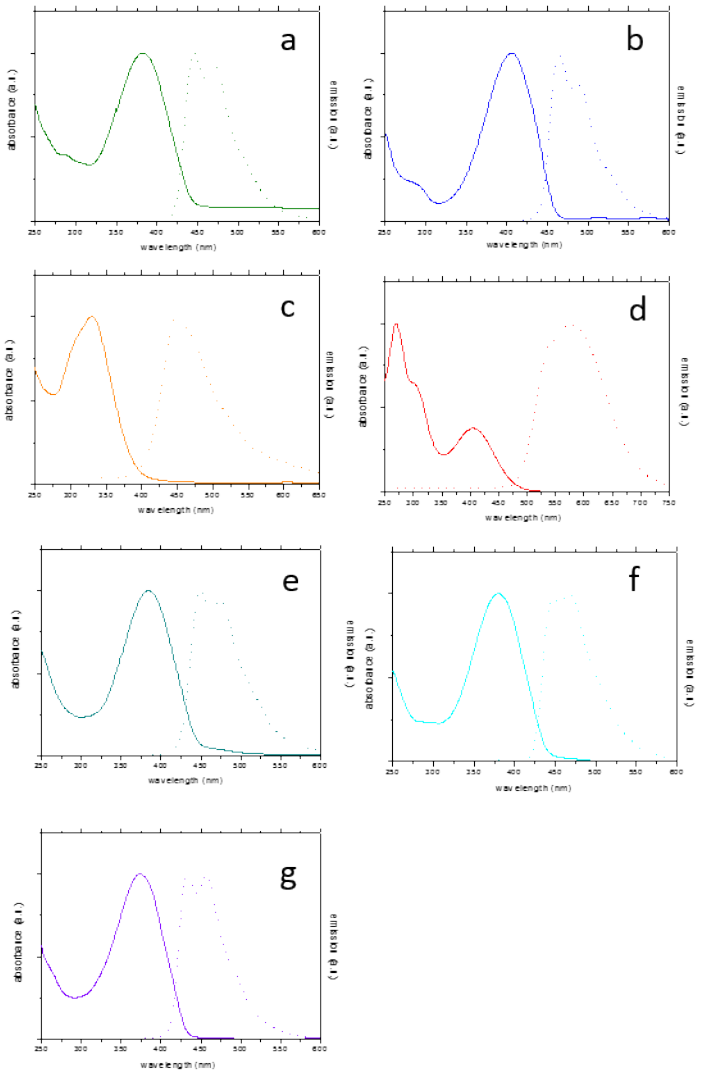

Figure S01: Normalized UV-Vis absorption and photoluminescence spectra of aromatic precursors in chloroform: (a) **ABT**, (b) **AOO** (c) **AXX** (d) **ACO**, (e) **AMeOMeO**, (f) **AMeOCF$_3$**, (g) **ACF$_3$CF$_3$**.

"Substituted core" "Substituted wings"	λ_{abs} (nm)	λ^{em}0-0 (nm)	Stokesshift
ABT	382	445	0.46
AOO	406	464	0.38
AXX	329	448	1.00
ACO	406	540	0.75
AMeOMeO	385	449	0.46
AMeOCF$_3$	379	448	0.50
ACF$_3$CF$_3$	372	433	0.47

Table S01: Absorption, emission and Stokes shift values of all aromatic compounds.

2. Crystallographic Information about **QOO.**

QOO	
Formula	$C_{46}H_{64}O_4S_2$
Fw	745,13
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	8.972 (2)
b (Å)	17.266 (4)
c (Å)	14.260 (5)
α (deg)	90.00
β (deg)	94.66 (3)
γ (deg)	90.00
V (Å^3)	2201.9 (12)
T (K)	296 (2)
Z	4
F(000)	804
P	1.121
M	1.39
cristalsize (mm^3)	0.30*0.08*0.08
θ_{max} (deg)	50.04
Total reflections Collected	4958
Rint	0.0578
No. Unique	2115
No. With I> 2σ(I)	1316
Refined parameters	243
Restraints	0
Final R indices [I> 2σ(I)]	R_1 = 0.0844w R_2 = 0.2102
R indices (all data)	R1 = 0.1343w R2 = 0.2427
Δρ [eÅ3]	(-) 0.274, 0.438

Figure S02: Crystallographic Information and structure refinement of **QOO**.