Supporting Information

Anthacene and pyrene tricyanofurane derivatives for second-order non-linear optics

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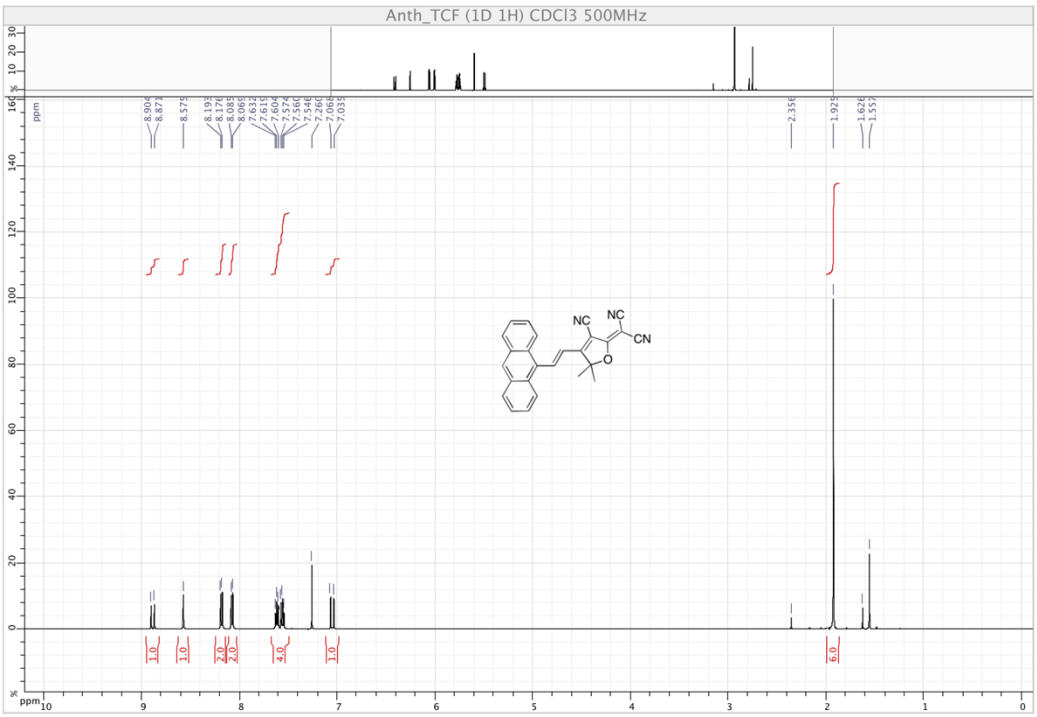

Figure S1. [1]H-NMR spectrum of **Anth_TCF**.

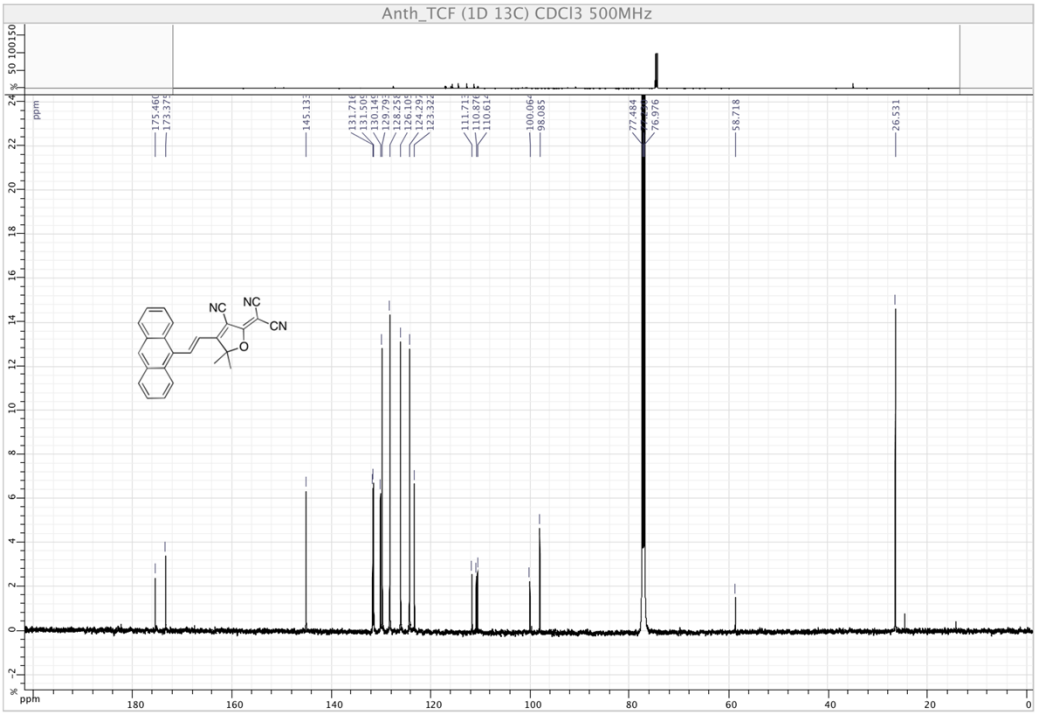

Figure S2. [13]C-NMR spectrum of **Anth_TCF**.

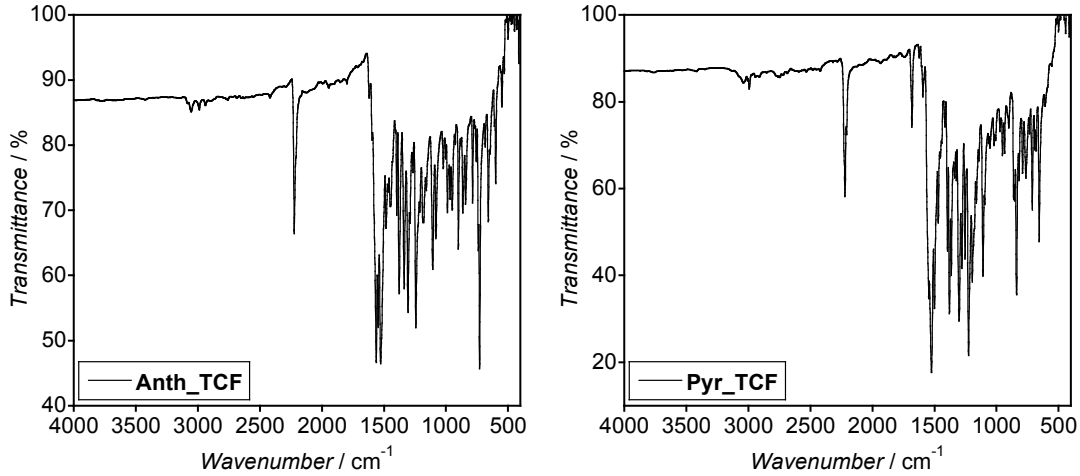

Figure S3. FT-IR spectra of **Anth_TCF** (*left*) and **Pyr_TCF** (*right*).

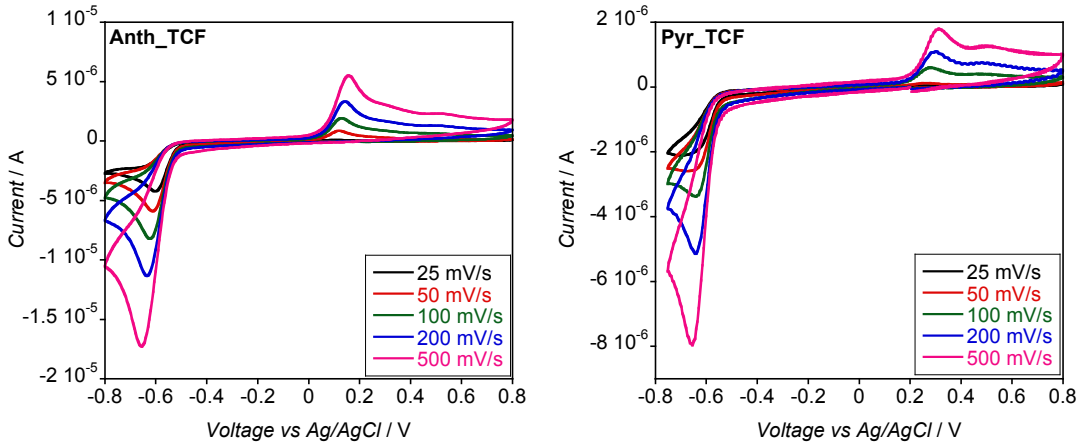

Figure S4. Cyclic voltammetry traces at different scan rates of **Anth_TCF** (*left*) and **Pyr_TCF** (*right*), where an irreversible reduction trace can be observed.

Supporting Information Tables

Table S1. TD-DFT calculated energies and compositions of the first six singlet electronic transitions of **Anth_TCF** and **Pyr_TCF** at B3LYP/6-31G(d) level of theory.

Compound	State	Composition[a]		Δ*E* (eV / nm)[b]	*f*[c]
Anth_TCF	1	HOMO → LUMO	100 %	2.0479 / 605.41	0.6307
	2	HOMO–1 → LUMO HOMO → LUMO+1	67 % 32 %	3.0413 / 407.67	0.2920
	3	HOMO–2 → LUMO HOMO → LUMO+3	95 % 4 %	3.2140 / 385.76	0.0641
	4	HOMO–1 → LUMO HOMO → LUMO+1	30 % 65 %	3.2507 / 381.41	0.0587
	5	HOMO–4 → LUMO	98 %	3.5190 / 352.33	0.0109
	6	HOMO–4 → LUMO HOMO–1 →LUMO+2 HOMO → LUMO+2	89 % 2 % 6 %	3.8862 / 319.04	0.2748
Pyr_TCF	1	HOMO → LUMO	100 %	2.1996 / 563.66	1.4233
	2	HOMO–2 → LUMO HOMO–1 → LUMO HOMO → LUMO+1	10 % 85 % 3 %	2.8854 / 429.69	0.2564
	3	HOMO–2 → LUMO HOMO–1 → LUMO HOMO → LUMO+1	84% 9 % 2 %	3.1111/ 398.52	0.0467
	4	HOMO–3 → LUMO	95 %	3.5225 / 351.98	0.0790
	5	HOMO–4 → LUMO HOMO → LUMO+1 HOMO–1 → LUMO	21 % 73 % 2 %	3.6214 / 342.36	0.0833
	6	HOMO–4 → LUMO HOMO →LUMO+1 HOMO–1 → LUMO HOMO–1 → LUMO+2 HOMO → LUMO+2 HOMO → LUMO+3	68 % 16 % 2 % 2 % 2 % 4 %	3.7945 / 326.75	0.1347

[a]Compositions of electronic transitions are expressed in terms of contributing excitations between ground state Kohn–Sham molecular orbitals. [b]Transition energy from the ground state to the excited state. [c]Oscillator strength.