Supporting information for
Photophysical and Semiconducting Properties of the Isomeric Triphenylimidazole Derivatives with Benzophenone Moiety

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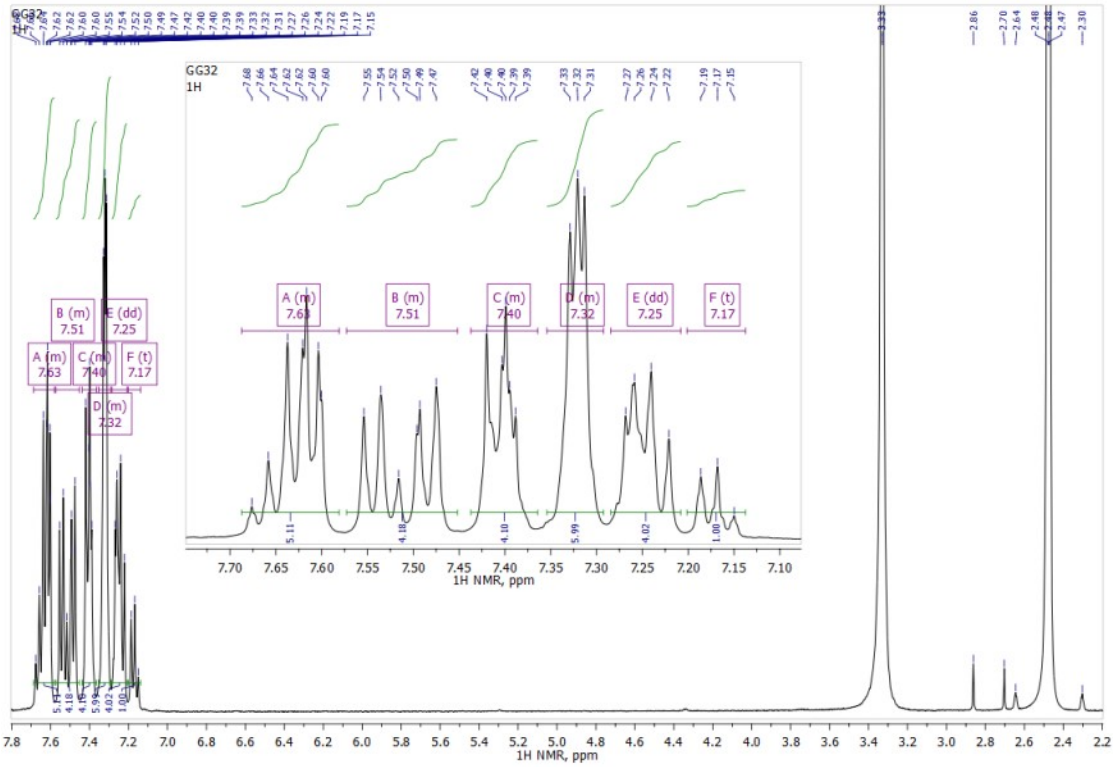


Figure S1. [1]H NMR spectrum of the compound **1**.

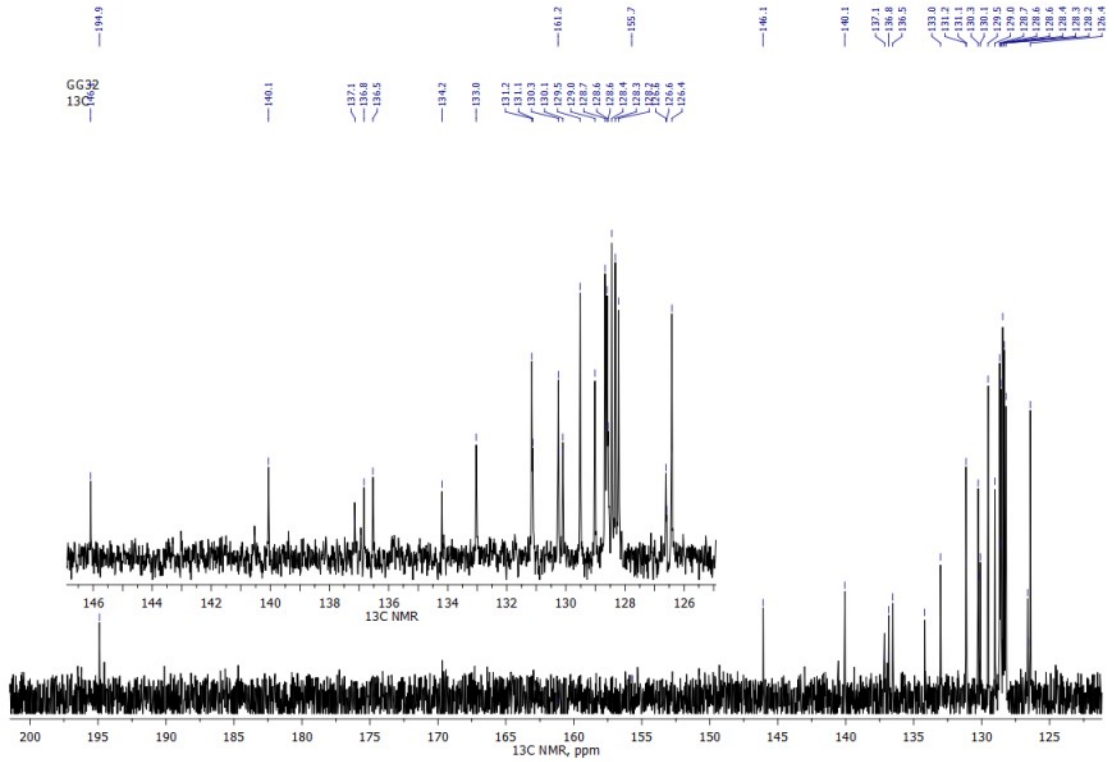


Figure S2. [13]C NMR spectrum of the compound **1**.

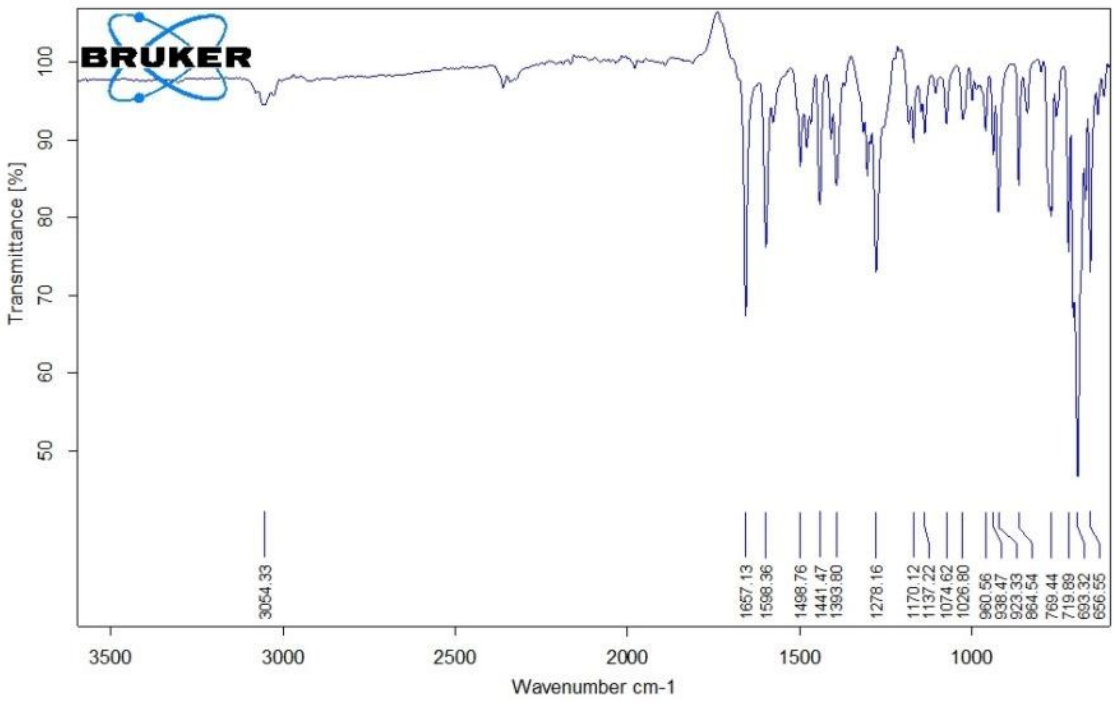


Figure S3. IR spectrum of of the compound **1**.

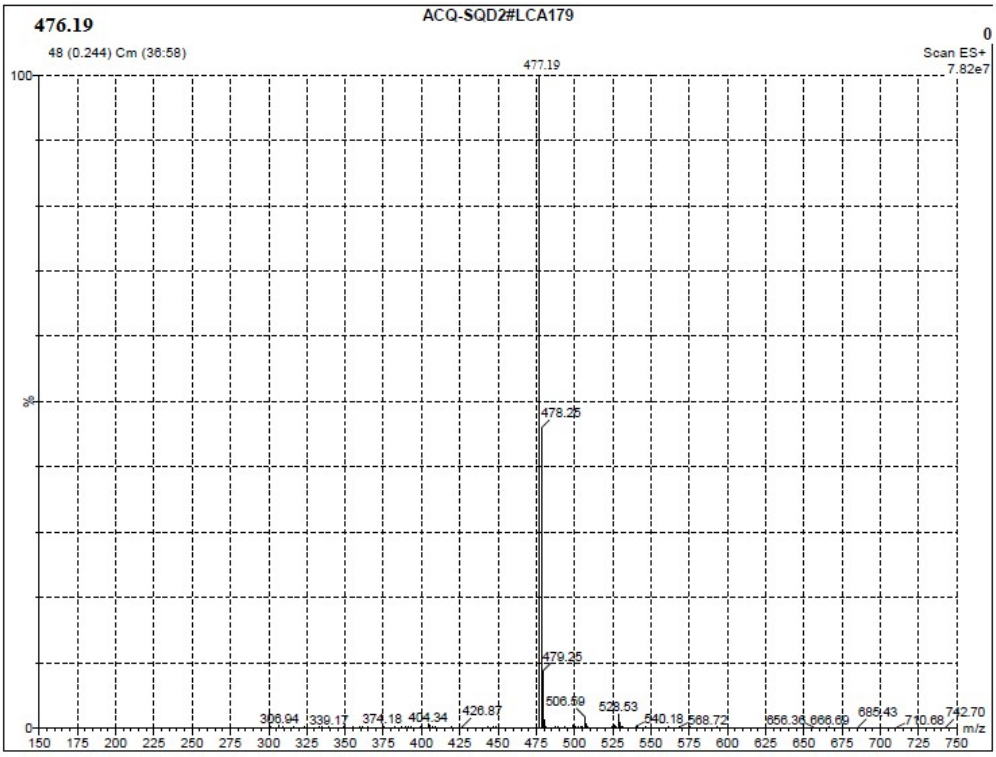


Figure S4. MS spectrum of compound **1**.

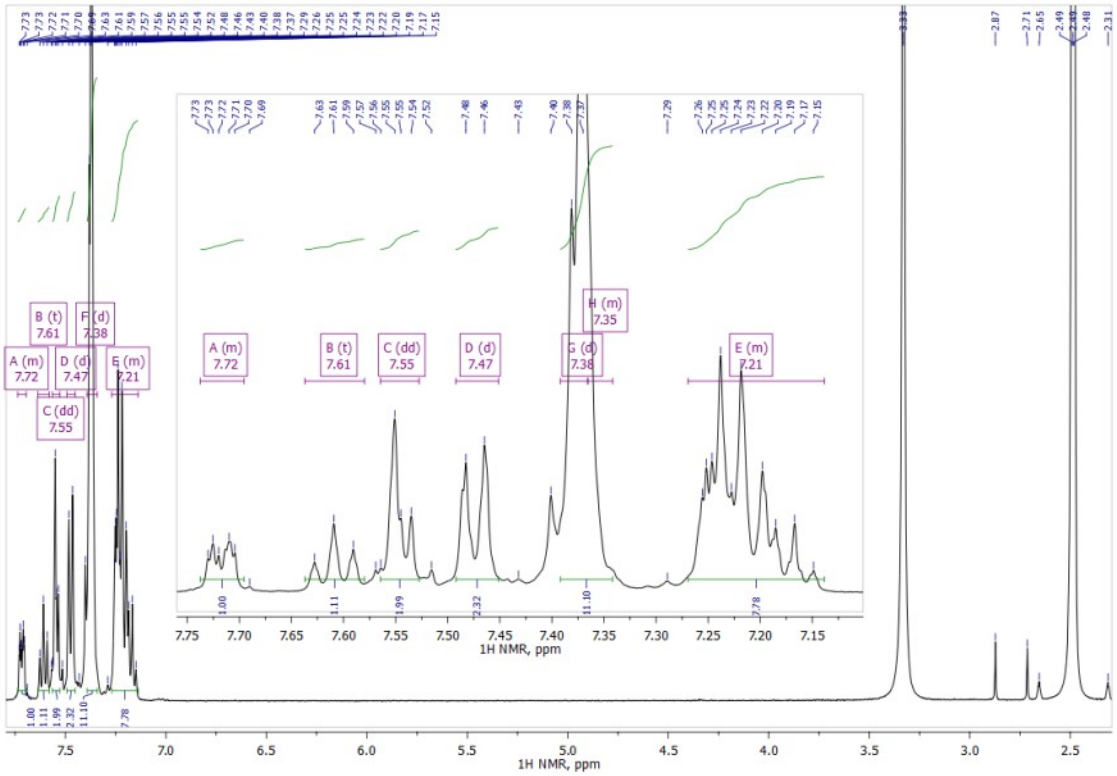


Figure S5. ^{1}H NMR spectrum of the compound **2**.

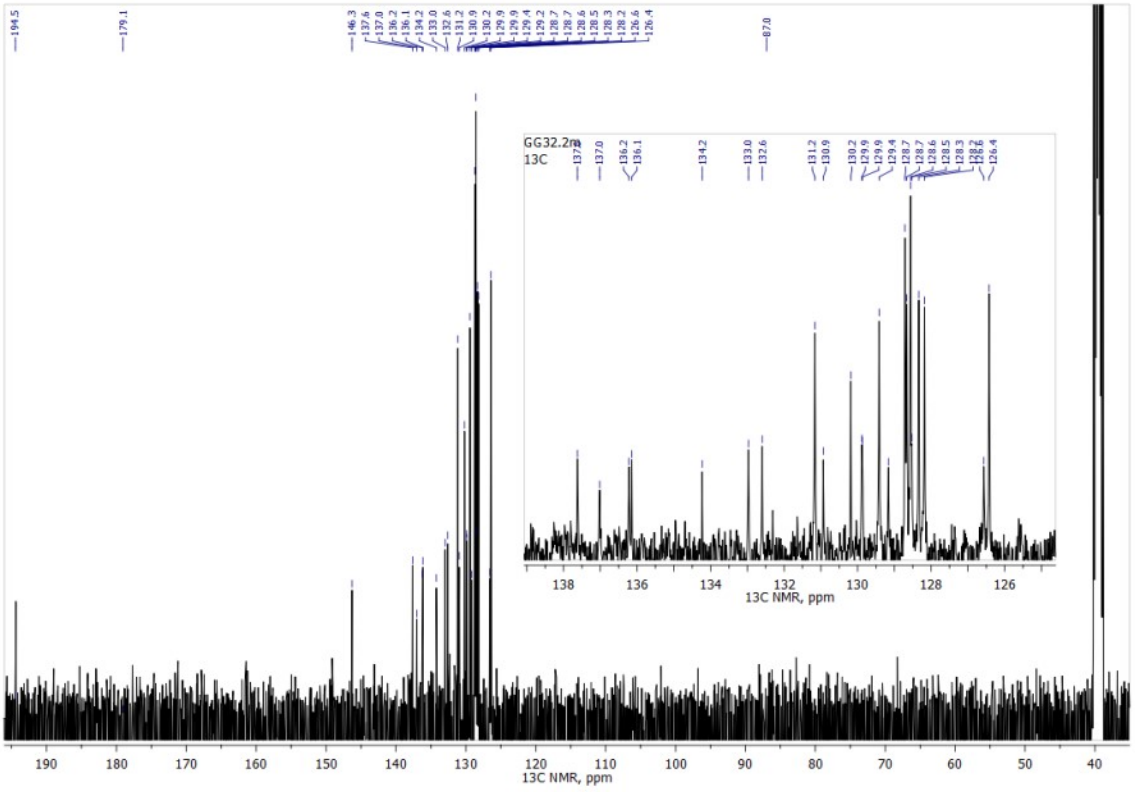


Figure S6. ^{13}C NMR spectrum of the compound **2**.

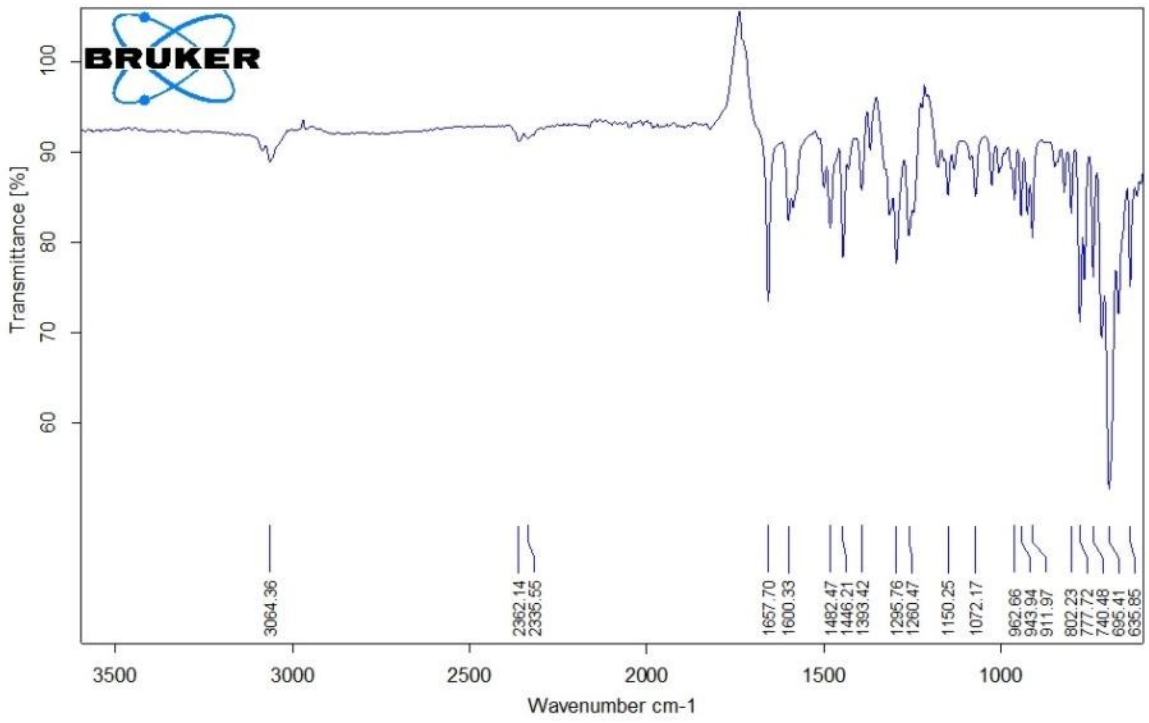


Figure S7. FT-IR spectrum of of the compound **2**.

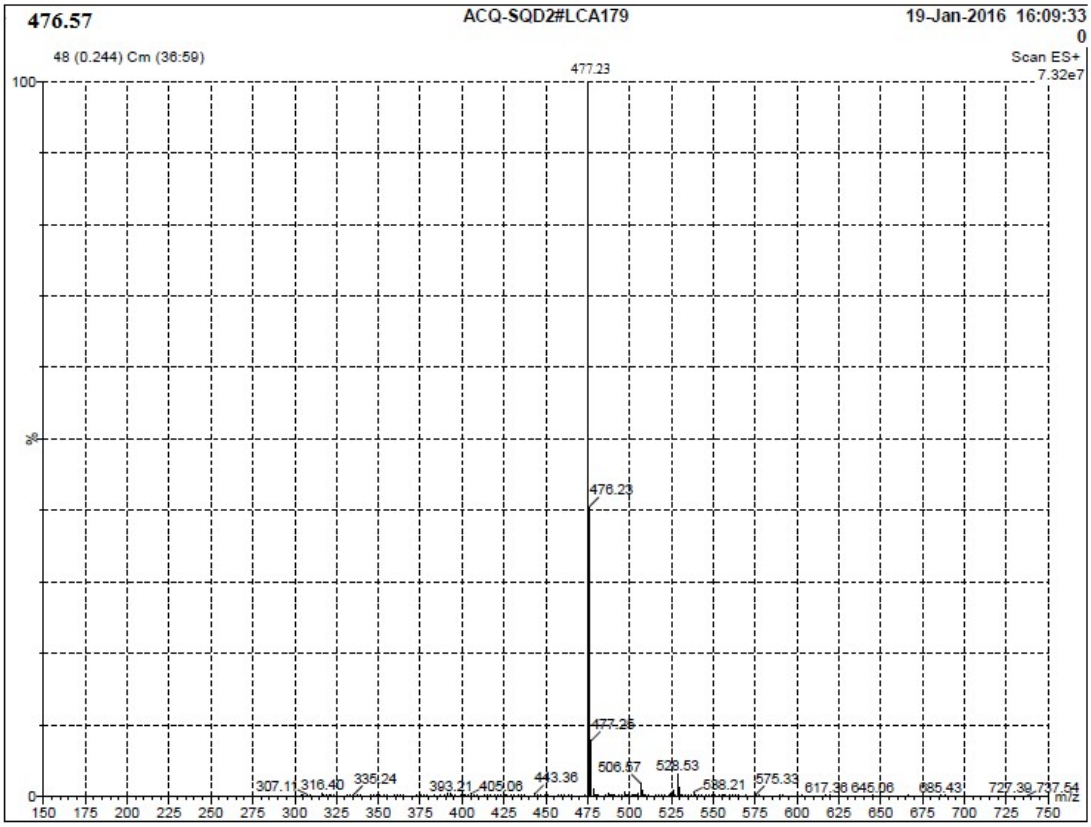
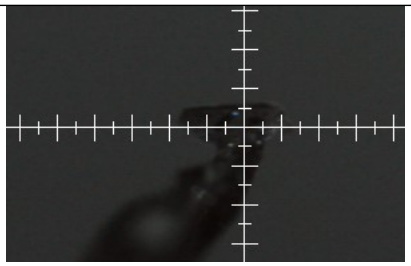
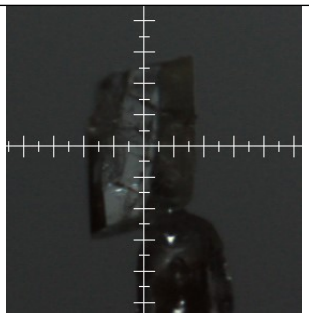


Figure S8. MS spectrum of compound **2**.

Table S1. Crystallographic and refinement data of **1** and **2**.

Compound	1	2
Crystal image on the needle		
CCDC deposition number	2061642	2061645
Empirical formula	$C_{34}H_{24}N_2O$	$C_{34}H_{24}N_2O$
Crystal dimensions (mm)	0.190 x 0.170 x 0.050	0.480 x 0.300 x 0.110
Crystal System	monoclinic	triclinic
Space group	$P2_1/n$ (#14)	P-1 (#2)
Z value	4	
Unit cell lengths (Å)	a = 9.37(2) b = 21.01(4) c = 13.22(3)	a = 10.211(12) b = 10.579(12) c = 12.370(13)
Unit cell angles (deg)	β = 102.98(3)	α = 99.13(2) β = 99.02(2) γ = 92.7263(10)
Cell volume (Å^3)	2536(10)	1299(3)
Density (g/cm^3)	1.248	1.218
R-factor[a]	0.0877	0.0589
wR2[b]	0.2388	0.1772
Temperature (K)	293	293

a- $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$

b- $wR2 = [S (w (Fo^2 - Fc^2)^2)/ S w(Fo^2)^2]^{1/2}$

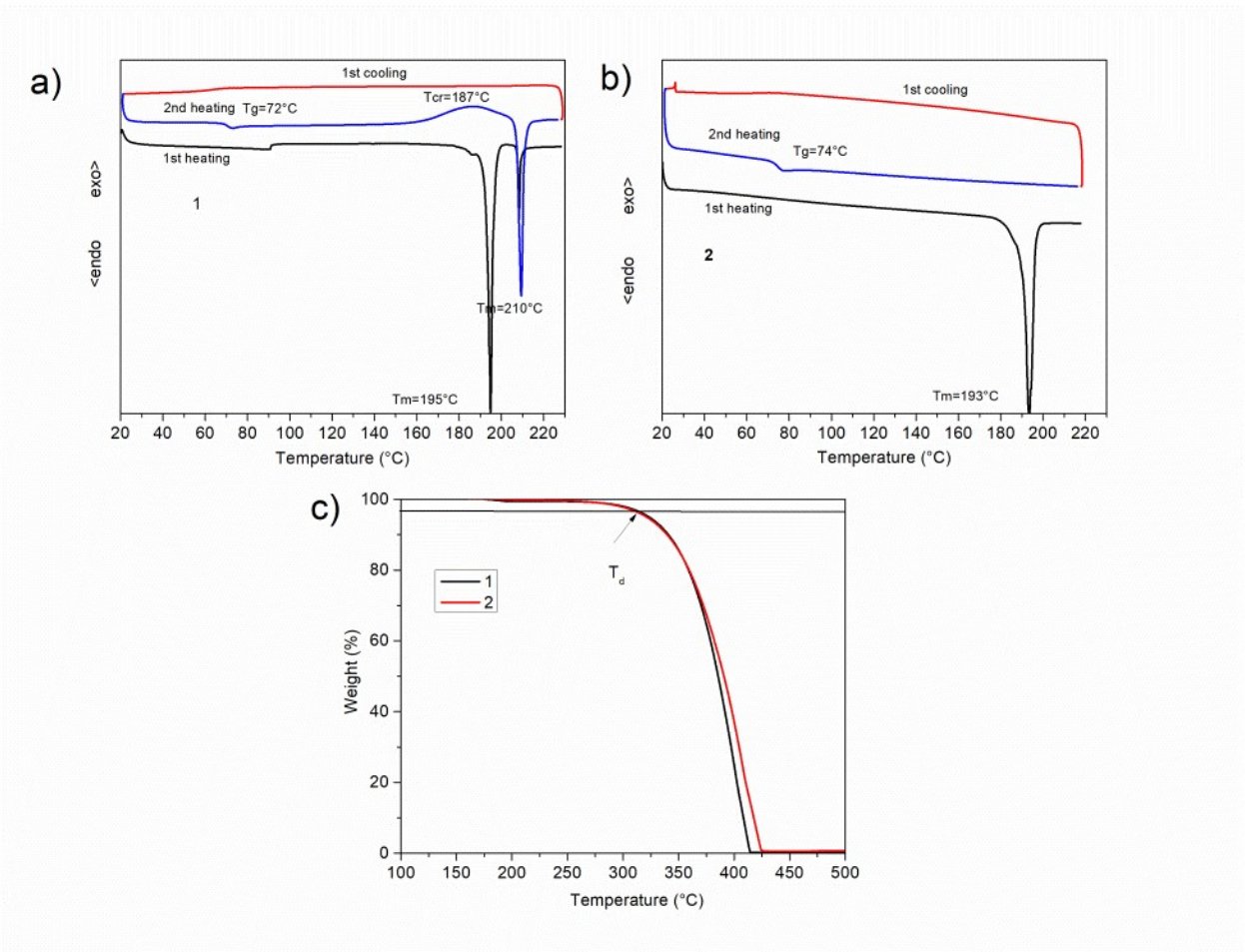


Figure S9. Thermal properties of 1 and 2: a) DCS of 1; b) DCS of 2; c) TGA of **1** and **2**.

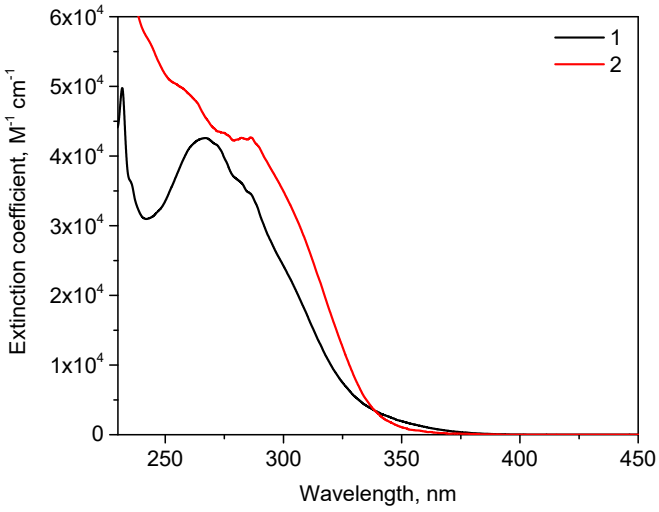


Figure S10. UV-vis spectra with extinction coefficients of **1** and **2** in THF. Concentration of the samples was 2.1×10^{-5} M.

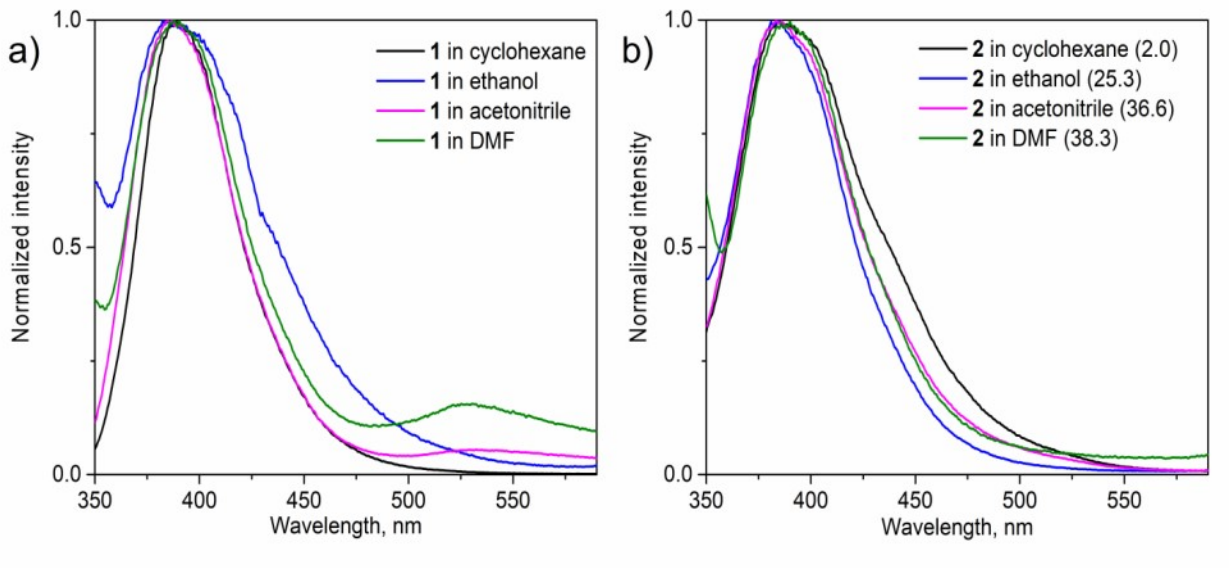


Figure S11. Solvatochromic effect on fluorescence spectra (a) for **1** and (b) for **2** in various organic solvents (c ~10^{-6} M, excitation was 310 nm).

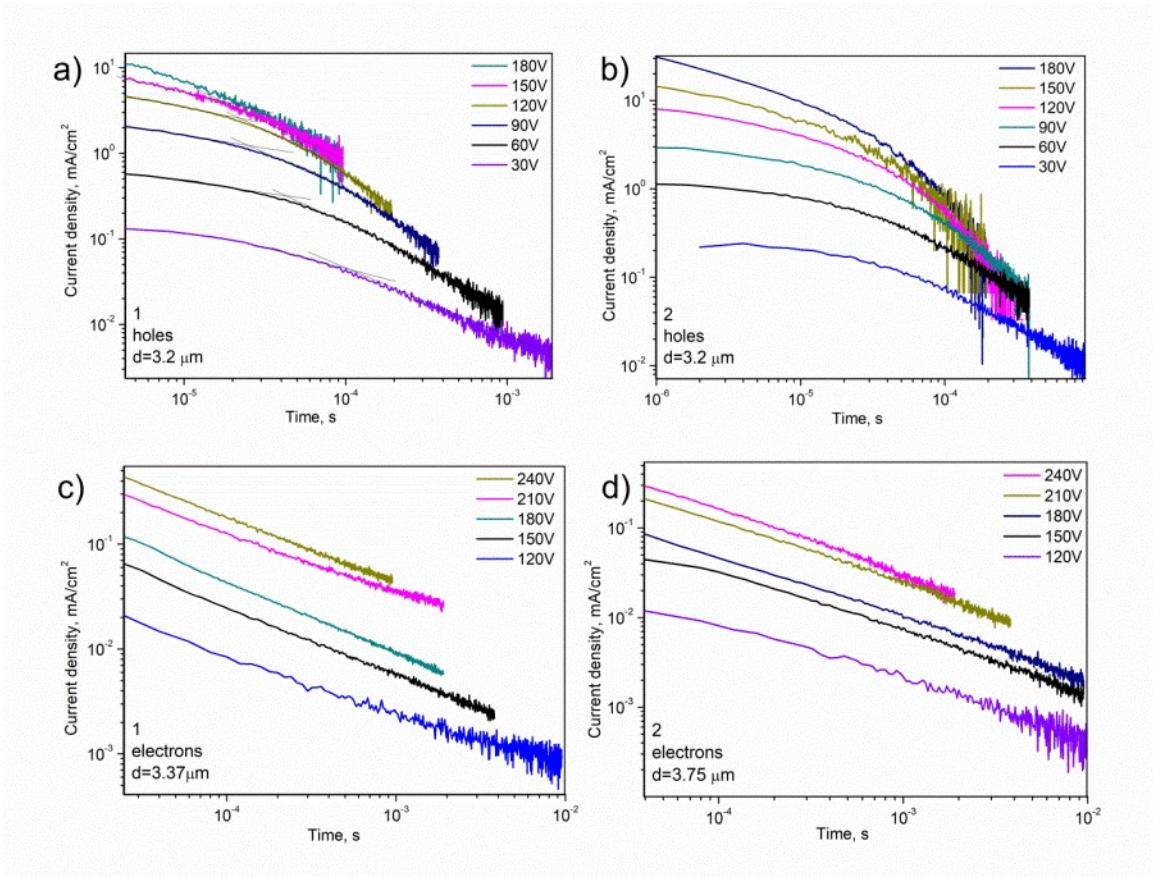


Figure S12. ToF pulses at the external electric fields of the transition of holes (a and b) and electrons (c and d) for the layers of 1 and 2, respectively

Table S2. Calculated molecular volumes, isotropic polizabilities and static dielectric constants of the corresponding materials

Compound	V, Å^{-3}	$R_{A,\,D}$, Å	A, Å^{-3}	ε_{st}
1	513.5	6.0	82.24	2.89
2	513.5	6.0	82.25	2.89

Table S3. Distances ($d_{D\text{-}D}/d_{A\text{-}A}$) between the neighbouring donor and acceptor moieties, intermolecular interaction ($-E_i$), total reorganization energies (λ_h/λ_h), coupling integrals ($|H_h|/|H_e|$), Gibbs free energies ($\Delta G_h/\Delta G_h$) and hoping probabilities (P_h/P_e) at F=0.

Compound 1: λ_h = 381 meV; λ_e = 394 meV					
Pathway	$d_{D\text{-}D}/d_{A\text{-}A}$, Å	$-E_i$, kJ mol^{-1}	$\|H_h\|/\|H_e\|$, meV	$\Delta G_h/\Delta G_h$, meV	P_h/P_e
1D1	6.18/13.2	122.1	19.7/0.10	296/404	$5.9\times10^{-3}/5.9\times10^{-6}$
1D2	4.40/15.6	110.6	54.6/3.5	215/418	$0.35/2.3\times10^{-3}$
1D3	12.48/9.75	40.6	0.1/7.5	398/370	$1.9\times10^{-23}/6.4\times10^{-16}$
1D4	9.86/11.5	19.8	57.7/22.9	372/390	$3.9\times10^{-21}/6.8\times10^{-19}$
Compound 2: λ_h = 372 meV; λ_e = 446 meV					
2D1	4.77/10.64	102.6	56.5/4.0	258/402	$0.92/5.3\times10^{-5}$
2D2	4.68/14.7	94.6	9.9/0.85	253/434	$1.3\times10^{-3}/2.9\times10^{-8}$
2D3	10.1/11.5	37.3	1.3/2.2	373/16	$2.6\times10^{-12}/3.4\times10^{-12}$
2D4	12.3/14.3	6.5	71.7/0.05	417/432	$5.9\times10^{-20}/4.0\times10^{-26}$