

Electronic Supplementary Information

Aggregation-induced emission of diarylamino- π -carborane triads: Effects of Charge transfer and π -conjugation

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Figures

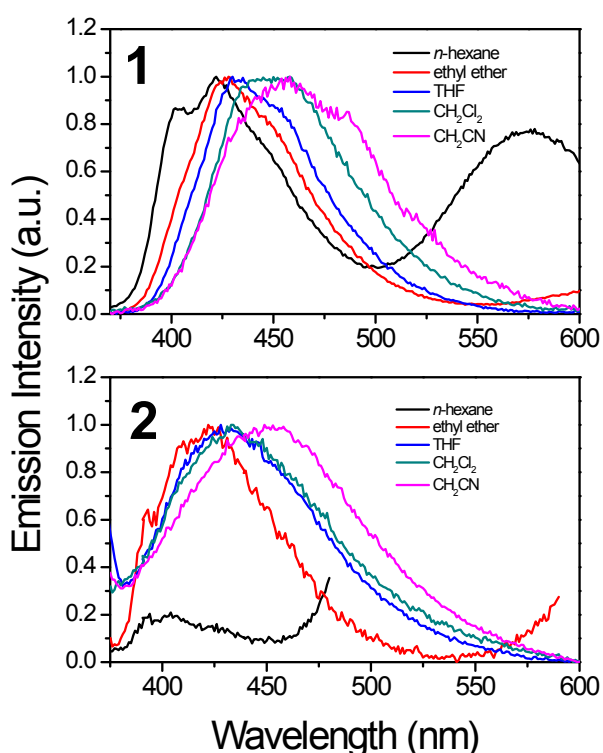


Fig. S1 emission spectra of **1** and **2** in various solvents.

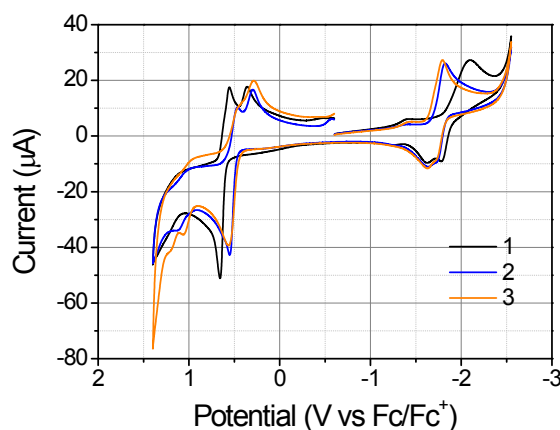


Fig. S2 Cyclic voltammograms of **1**, **2** and **3**.

Tables

Table S1. Maxima wavelength (nm) for the CT emission of **1**, **2**, and **3** measured in various solvents

solvents	1	2	3
<i>n</i> -hexane	393	404	405
Ethyl ether	412	421	418
THF	423	430	432
CH ₂ Cl ₂	433	437	439
CH ₃ CN	459	451	459

Table S2. Maxima wavelength (nm) for the AIE emission of **1**, **2**, and **3** measured in various solvents

solvents	1	2	3
<i>n</i> -hexane	577	570	577
cyclohexane	581	577	563
dibutyl ether	622	652	665
ethyl ether	650	695	-
CHCl ₃	677	703	-
ethyl acetate	683	759	-
CH ₃ CN	682	-	-

Table S3. Energies (eV) of orbitals calculated by B2LYP/6-31G(d,p) for **1**, **2** and **3**.

orbitals	1	2	3
L+3		-1.121	-1.228
L+2	-1.174	-1.281	-1.249
L+1	-1.375	-1.327	-1.388
LUMO	-1.430	-1.503	-1.624
HOMO	-5.344	-5.158	-5.072
H-1	-5.375	-5.169	-5.075
H-2	-6.201	-6.076	-5.968
H-3		-6.097	-5.984