Electronic Supplementary Information

Synthesis, Structure, and Property of 5,6,11,12-Tetraarylindeno[1,2-*b*]fluorenes as Donors for Organic Photovoltaic Devices

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General Methods

All chemicals and reagents were used without purification from commercial sources. Solvents for chemical analysis and reaction were purified by distillation with drying equipment. NMR spectra were measured in $CDCl_3$ through Varian (Utility 400) spectrometer at for ^1H NMR (400 MHz) and ^{13}C (100 MHz) respectively. Optical absorption were conducted through JASCO V-670 spectrophotometer. The electrochemical properties of all the products were measured by cyclic voltammetry (using CHI619B potentiostat). The measurements of oxidation potentials were conducted in dried dichloromethane (for 1.0 mM) with 0.1 M tetrabutylammonium hexafluorophosphate ($^nBuNPF_6$) as supporting electrolyte. The measurements of reduction potentials were conducted in dried tetrahydrofuran (for 1.0 mM) with 0.1 M tetrabutylammonium perchlorate ($^nBuNClO_4$) as supporting electrolyte, and degassed by argon prior to conduct the experiment. A glassy carbon electrode was used as working electrode and a platinum wire was used as counter electrode. And all the potentials were recorded versus Ag/AgCl as a reference electrode, further calibrated with the ferrocene/ferrocenium (Fc/Fc^+) redox couple (0.47 eV in dichloromethane/ $^nBuNPF_6$ and 0.633 eV in tetrahydrofuran/$^nBuNClO_4$).

All the mass spectra were recorded by National Taiwan University Mass Spectrometry-based Proteomics Core Facility in MALDI-TOF mode without using matrix. Melting temperature was measured by Fargo Instrument MP-1D. Theoretical calculations with density functional theory (DFT) and time-dependent DFT (TD-DFT) were conducted in gaseous state at a B3LYP/6-311g (d) level by ALPS (Advanced Large-scale Parallel Supercluster, National Center for High-Performance Computing).

All the crystals for single x-ray diffraction analysis are obtained by bilayer method ($CHCl_3$/ hexane).

X-ray Crystallography: Crystallographic data were carried out at 200(2) K on a Oxford Gemini A CCD diffractometer using with Mo-Kα radiation (λ = 0.71073Å). Cell parameters and data reduction were retrieved and refined manipulating CrysAlis Pro software on all reflections. The structures were solved and refined with SHELXL programs. The hydrogen atoms were included in calculated positions and refined using a riding mode.

Synthesis

Synthesis of 5,11-diphenylindeno[1,2-b]fluorene-6,12-dione (**2**)

Adding **1** (500 mg, 0.950 mmol) into mixed solvent of acetic acid : sulfuric acid = 5.00 mL : 2.00 mL with stirring. Then heat the solution up to refluxing temperature

for 2.5 hours. When the solution was cooled down to room temperature, slowly poured the acidic solution into iced water, filtered and washed with methanol and diethyl ether to get orange solid **2**[1] (0.361 g, 87.4%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.58-7.59 (m, 6H), 7.50 (d, J =6.4 Hz, 2H), 7.42-7.44 (m, 4H), 7-14-7.17 (m, 4H), 6.27 (d, J=6.4 Hz, 2H).

Synthesis of 5,6,11,12-tetraphenylindeno[1,2-b]fluorene (**TAInF1**)

n-Butyllithium (1.6 M solution in hexane, 28.80 mL, 46.00 mmol) was added dropwise into a solution of bromobenzene (4.70 mL, 46.0 mmol) in 50 mL dried tetrahydrofuran (THF) under -78 °C under argon atmosphere and stirred for 30 mins. Then a suspension of **2** (2.00 g, 4.60 mmol) in 50 mL dried THF was transferred into the solution under -78 °C through syringe. When the suspension of **2** was totally transferred into the solution containing lithium reagent, the mixture was warmed up to room temperature and stirred for 12 hours. 200 mL of water was added into the mixture to quench unreacted lithium reagent. Then 30 mL of brine was added into the mixture then extracted with 50 mL of EA for 3 times. The organic part was dried over magnesium sulfate ($MgSO_4$). Then the diol compound was obtained from rotary evaporation. Then the crude product was mixed with tin(II) chloride (3.49 g, 18.4 mmol) and suspended in 200 mL toluene. The suspension was heated up to 120 °C and stirred for 5 hours. Then the solution was cooled down to room temperature and filtered to remove tin(II) chloride. The solid was washed with chloroform (200 mL) and the solution of filtrate was removed to recover the crude product. The crude product was purified by column chromatography. Brown solid was obtained in 9 % yield (230 mg). Melting point > decompose temperature. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13-7.15, (m, 4H), 7.06-7.10 (m, 6H), 6.97-7.00 (m, 6H), 6.88-6.90 (m, 4H), 6.80 (td, *J*=8.0, 0.8 Hz, 2H), 6.69, (d, *J* = 7.2 Hz, 2H), 5.94 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 126 MHz) δ 147.17, 145.90, 138.60, 136.98, 136.29, 134.45, 133.60, 129.34, 128.90, 127.93, 127.37, 127.23, 127.03, 126.44, 123.60, 122.23. HRMS (m/z, MALDI, no matrix) calcd for $C_{44}H_{28}$: 556.2186, found 556.2144.

Synthesis of 5,11-diphenyl-6,12-di-p-tolylindeno[1,2-b]fluorene (**TAInF2**)

n-Butyllithium (1.6 M solution in hexane, 28.80 mL, 46.00 mmol) was added dropwise into a solution of 4-bromotoluene (4.67 mL, 46.0 mmol) in 50 mL dried THF under -78 °C under argon atmosphere and stirred for 30 mins. Then a suspension of **2** (2.00 g, 4.60 mmol) in 50 mL dried THF was transferred into the solution under -78 °C through syringe. When the suspension of **2** was totally transferred into the

[1] Samuel M.; Maria B.; Wang, Z. Y. *Org. Lett.,* **2002**, *4*, 2157.

solution containing lithium reagent, the mixture was warmed up to room temperature and stirred for 12 hours. 200 mL of water was added into the mixture to quench unreacted lithium reagent. Then 30 mL of brine was added into the mixture and extracted with 50 mL of EA for 3 times. The organic part was dried over magnesium sulfate ($MgSO_4$). Then the diol compound was obtained from rotary evaporation. Then the crude product was mixed with tin(II) chloride (3.49 g, 18.4 mmol) and suspended in 200 mL toluene. The suspension was heated up to 120 °C and stirred for 5 hours. Then the solution was cooled down to room temperature and filtered to remove tin(II) chloride. The solid was washed with chloroform (200 mL) and the solution of filtrate was removed to recover the crude product. The crude product was purified by column chromatography. Brown solid was obtained in 47 % yield (1.27 g). Melting point > decompose temperature. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.11-7.13 (m, 6H), 7.03-7.10 (m, 4H), 6.72-6.80 (m, 12H), 6.61 (td, *J* = 7.6, 0.8 Hz, 2H), 5.96 (d, *J* = 7.6 Hz, 2H), 2.23 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.16, 145.87, 138.54, 137.19, 137.07, 136.16, 135.97, 133.66, 131.40, 129.41, 128.77, 127.87, 127.85, 126.93, 126.88, 123.58, 122.21, 21.17. HRMS (m/z, MALDI, no matrix) calcd for $C_{46}H_{32}$: 584.2499, found 584.2489.

Synthesis of 2,2'-(5,11-diphenylindeno[1,2-b]fluorene-6,12-diyl)dithiophene (**TAInF3**)

n-Butyllithium (1.6 M solution in hexane, 28.80 mL, 46.00 mmol) was added dropwise into a solution of thiophene (3.69 mL, 46.0 mmol) in 50 mL dried THF under -78 °C under argon atmosphere and stirred for 30 mins. Then a suspension of **2** (2.00 g, 4.60 mmol) in 50 mL dried THF was transferred into the solution under -78 °C through syringe. When the suspension of **2** was totally transferred into the solution containing lithium reagent, the mixture was warmed up to room temperature and stirred for 12 hours. 200 mL of water was added into the mixture to quench unreacted lithium reagent. Then 30 mL of brine was added into the mixture and extracted with 50 mL of EA for 3 times. The organic part was dried over magnesium sulfate ($MgSO_4$). Then the diol compound was obtained from rotary evaporation. Then the crude product was mixed with tin(II) chloride (3.49 g, 18.41 mmol) and suspended in 200 mL toluene. The suspension was heated up to 120 °C and stirred for 5 hours. Then the solution was cooled down to room temperature and filtered to remove tin(II) chloride. The solid was washed with chloroform (200 mL) and the solution of filtrate was removed to recover the crude product. The crude product was purified by column chromatography. Brown solid was obtained in 13% yield (340 mg). Melting point >decompose temperature. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.17-7.24 (m, 10H), 7.10 (dd, *J* = 5.2, 0.8 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.85 (td, *J* = 6.8, 0.8 Hz, 2H),

6.61-6.65 (m, 2H), 6.57-6.59 (m , 2H), 6.39, (dd, J = 3.6, 2.8 Hz, 2H), 5.93, (d, J = 7.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 126MHz) δ145.83, 140.00, 138.53, 137.11, 136.81, 136.64, 135.27, 134.88, 129.09, 128.80, 128.08, 127.50, 127.28, 127.26, 126.66, 125.99, 123.71, 122.51. HRMS (m/z, MALDI, no matrix) calcd for $C_{40}H_{24}S_2$: 568.1314, found 568.1299.

Device fabrication and measurements, atomic force microscope, photoelectron spectrometer, and absorption spectrum.

The MoO_3, C_{70}, BCP, and Ag were purchased from Sigma-Aldrich. ITO-coated glass substrates with 10 Ω/sq were purchased form Luminescence Technology Corporation. The deposition of organic and metal thin film was performed in a thermal evaporator with a pressure lower than 5×10^{-6} torr, while the deposition rate was monitored by a quartz crystal microbalance (Sycon Instruments STM-2XM). After the deposition process, the devices were well encapsulated in a nitrogen-filled glove box. The pixel area of 0.04 cm^2 was defined by a shadow mask. For device characterizations, the current density versus voltage characteristics of organic photovoltaic devices (OPVs) were measured by a source meter (Keithley 2401) in the dark and under an AM 1.5G solar simulator (Newport 91160A) with an intensity of 100 mW/cm^2. For measuring the external quantum efficiency (EQE), a monochromator (Newport 74100) and lock-in amplifier (SRS SR830) were used to measure the value of EQE, which set the chopper's frequency at 250 Hz. Note that our measurement system exhibited an error of less than 5% as compared with the experimental short circuit current density (Jsc) and integration of the EQE. Atomic force microscope (AFM) images were performed by a Park System (XE-70) with a non-contact mode, while an NCHR-type cantilever was used to map the surface morphology of organic thin films. The HOMO levels of organic thin films were measured by a low-energy photoelectron spectrometer (Riken Keiki AC-2) and cyclic voltammetry method (CHI 619B). The LUMO levels of the organic materials were estimated by using a UV-visible spectrophotometer (Thermo Scientific Evolution 220) to measure the optical band-gap and then subtracting the HOMO levels to calculate it.

Table S1 Single crystal data of **TAInF1~3**

Compounds	**TAInF1**	**TAInF2**	**TAInF3**
Empirical formula	$C_{44}H_{28}$	$C_{46}H_{32}$	$C_{40}H_{24}S_2$
formula weight	556.66	584.72	568.71
crystal dimensions	0.42 x 0.07 x 0.05 mm^3	0.50 x 0.13 x 0.13 mm^3	0.30 x 0.10 x 0.05 mm^3
crystal system	triclinic	orthorhombic	triclinic
space group	$P\bar{1}$	$Pna2_1$	$P\bar{1}$
a (Å)	7.5970(4)	16.8864(4)	7.5051(7)
b (Å)	8.9994(4)	7.4906(2)	8.6296(7)
c (Å)	11.0344(5)	24.7447(7)	11.6509(11)
α (deg)	78.931(2)	90	73.729(5)
β (deg)	75.805(2)	90	77.669(4)
γ (deg)	83.409(2)	90	77.532(6)
cell volume $(Å)^3$	715.95(6)	3129.94(14)	697.78(11)
Z	1	4	1
density (calc) g/ cm^3	1.291	1.241	1.353
F(000)	292.0	1232.0	296.0
Temperature (K)	200	200	200
Wavelength (Å)	0.71073	0.71073	0.71073
no. of reflns collected	10507	17367	12387
no. of indep reflns (R_{int})	3262 (0.0645)	7089 (0.0352)	3193 (0.0658)
R(F), wR_2 [I>2σ(I)]	0.0504, 0.1131	0.0504, 0.1175	0.0167, 0.1647
R(F), wR_2 (all data)	0.0955, 0.1326	0.0692, 0.1276	0.1065, 0.1884

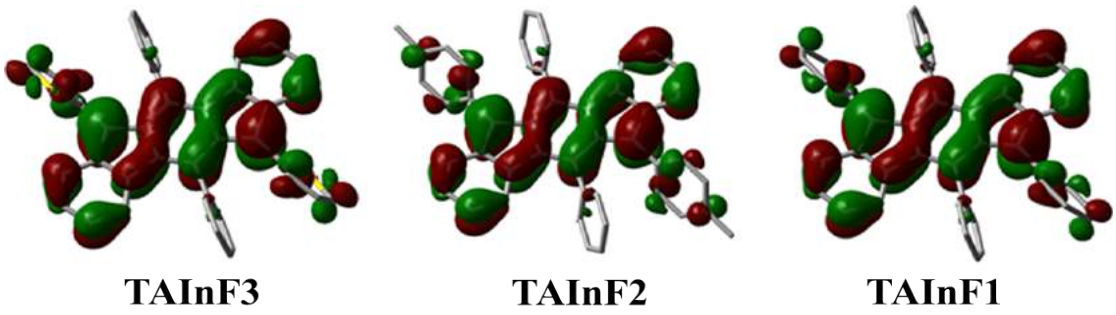

Figure S1 Singly occupied orbitals distribution of **TAInF1**~**TAInF3**

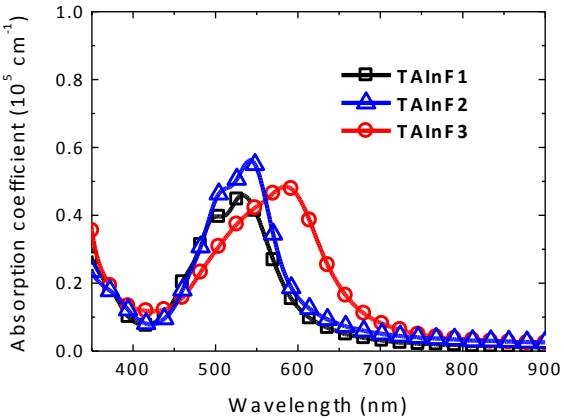

Figure S2 Absorption coefficient of **TAInF1** (square), **TAInF2** (triangle), and **TAInF3** (circle) thin films.

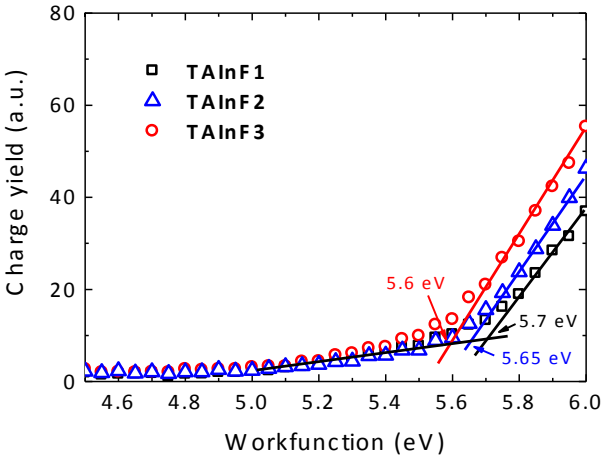

Figure S3 The workfunction of **TAInF1** (square), **TAInF2** (triangle), and **TAInF3** (circle) thin films by low-energy photoelectron spectroscopy.

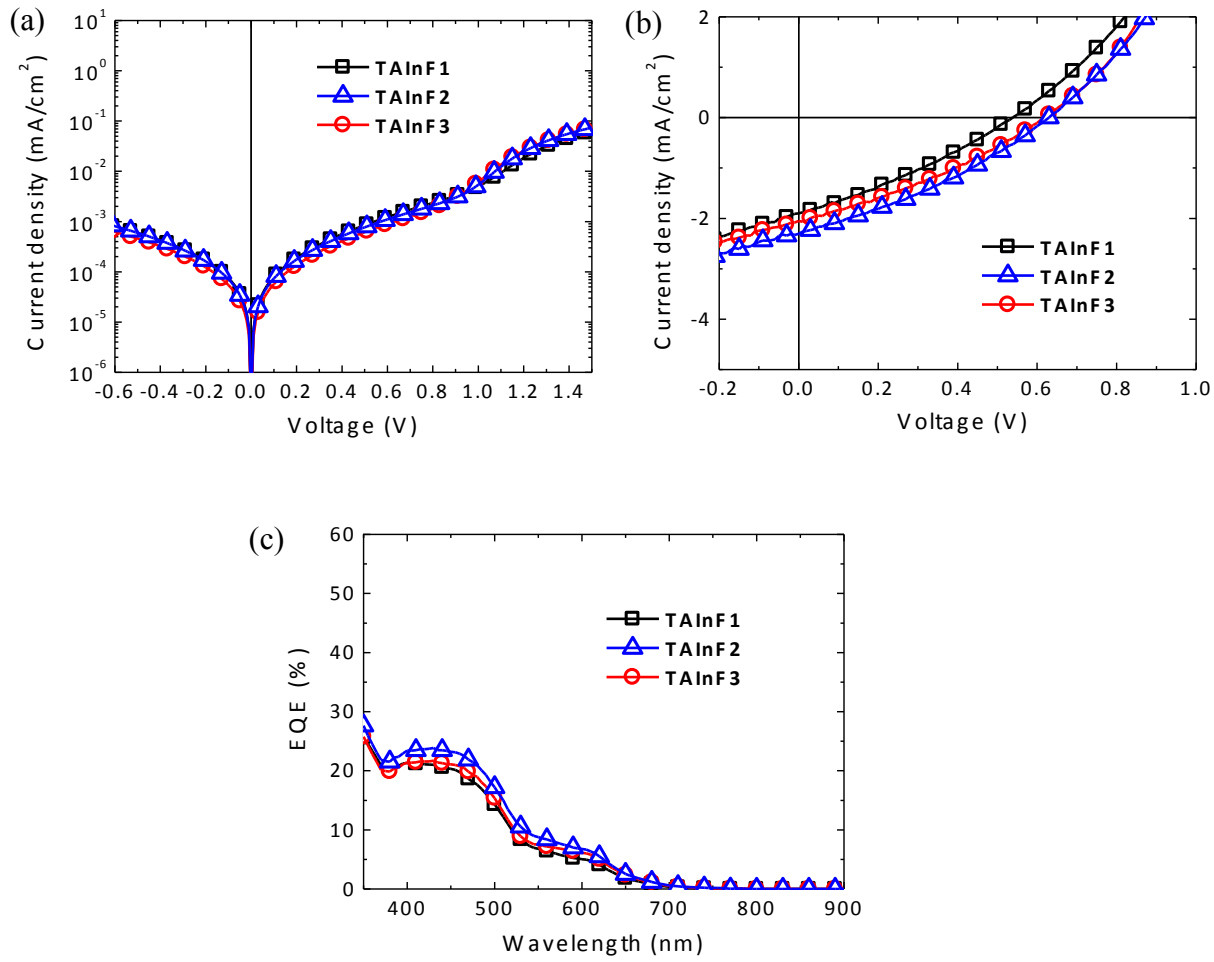

Figure S4 The device performances of planar **TAInF1** (square), **TAInF2** (triangle), and **TAInF3** (circle) OPVs of (a) dark, (b) light, and (c) external quantum efficiency.

Table S2 The bilayer-type device performances of **TAInF1:**C_{60}, **TAInF2:**C_{60}, and **TAInF3**:C_{60} bulk heterojunction OPVs with **TAInF1~3** (12 nm)/ C_{60} (50 nm).

Donor	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	R_S (Ω cm^{-2})	R_{SH} (kΩ cm^{-2})
TAInF1	0.54	1.90	30.51	0.31	7.00	0.41
TAInF2	0.63	2.30	32.22	0.47	6.30	0.50
TAInF3	0.62	2.05	31.96	0.41	6.38	0.49

Table S3 The device performances of **TP-IDF:**C_{70}, **DTDP-IDF:**C_{70}, and **DTLDP-IDF**:C_{70} bulk heterojunction OPVs with mixing ratio of 1:1 and 1:10.

Mixing ratio 1:1	**V_{OC} (V)**	**J_{SC} (mA cm^{-2})**	**FF (%)**	**PCE (%)**	**R_S (Ω cm^{-2})**	**R_{SH} (kΩ cm^{-2})**
TAInF1:C_{70}	0.90	2.37	22.89	0.49	4.87	0.32
TAInF2:C_{70}	0.91	2.00	21.25	0.39	6.20	0.33
TAInF3:C_{70}	0.81	2.97	25.38	0.62	6.02	0.28

Mixing ratio 1:10	**V_{OC} (V)**	**J_{SC} (mA cm^{-2})**	**FF (%)**	**PCE (%)**	**R_S (Ω cm^{-2})**	**R_{SH} (kΩ cm^{-2})**
TAInF1:C_{70}	0.97	6.27	28.09	1.71	6.20	0.33
TAInF2:C_{70}	0.94	8.62	35.90	2.91	7.06	0.22
TAInF3:C_{70}	0.80	6.55	32.37	1.71	6.18	0.17

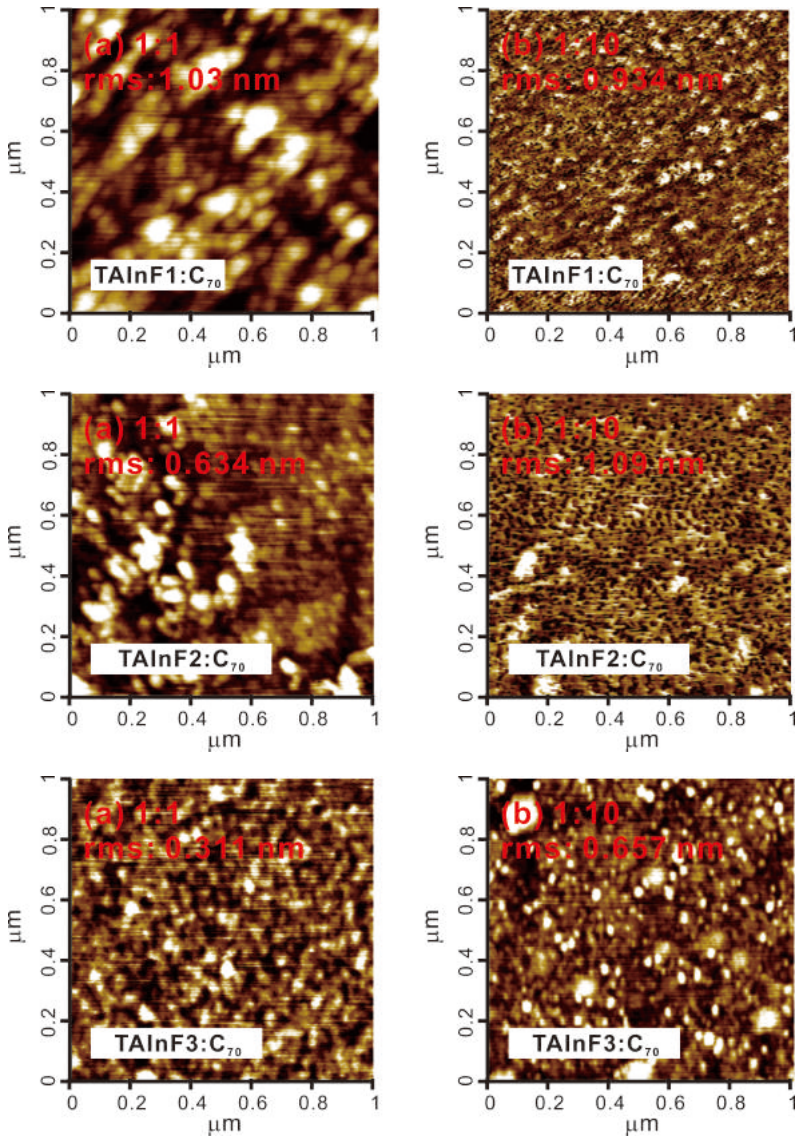

Figure S5 AFM images of 45 nm **TAInF1~3:**C_{70} with mixing ratio of (a) 1:1 and (b) 1:10 thin films.

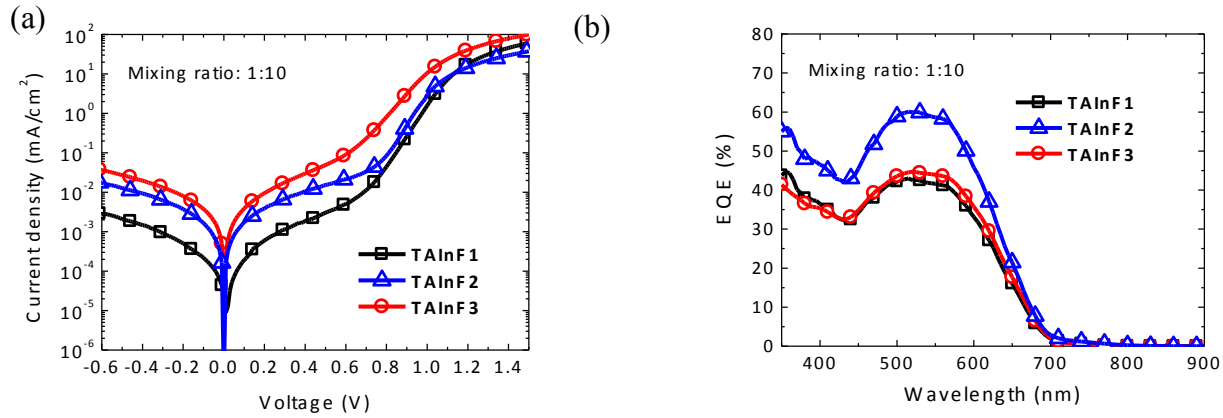

Figure S6 The device performances of bulk heterojunction **TAInF1** (square), **TAInF2** (triangle), and **TAInF3** (circle) OPVs with mixing ratio of 1:10 of (a) dark and (b) external quantum efficiency.

DFT calculation details

Density functional theory calculations were employed with Gaussian 09 package,[1] utilizing the B3LYP (and UCAM-B3LYP)[2-4] level of theory with Pople basis set 6-31G*[5-7] for all molecules in the gas phase. The energies and Cartesian coordinates of the optimized structures (B3LYP) are shown below.

Compound **TAInF1**

Sum of electronic and zero-point Energies=	-1692.981313
Sum of electronic and thermal Energies=	-1692.948486
Sum of electronic and thermal Enthalpies=	-1692.947542
Sum of electronic and thermal Free Energies=	-1693.047459

C	-1.16947600	0.88198900	0.01503200
C	0.09898200	1.40692900	0.03657200
C	0.56040100	2.80515300	0.08380500
C	-0.09279600	4.03452700	0.17950600
H	-1.17239300	4.09683900	0.22726500
C	0.66725400	5.21064600	0.22036600
H	0.15769700	6.16792800	0.29278000
C	2.06420400	5.17122600	0.17612300
H	2.63380700	6.09605000	0.21250400

C	2.73205900	3.94711900	0.09926600
H	3.81716700	3.90769100	0.08527900
C	1.98045600	2.77074400	0.05120300
C	2.42819800	1.37960600	0.02404500
C	1.30262000	0.55995100	0.02041900
C	-2.36666300	1.77632400	0.02002900
C	-3.11229000	1.97119200	1.19008600
H	-2.82844900	1.44520600	2.09717100
C	-4.20846000	2.83428300	1.19703400
H	-4.77603100	2.97613500	2.11285300
C	-4.57540100	3.51321300	0.03367800
H	-5.42973000	4.18490100	0.03999700
C	-3.83884800	3.32521300	-1.13764700
H	-4.11609800	3.85171600	-2.04733400
C	-2.74141200	2.46415600	-1.14327500
H	-2.16070400	2.32701400	-2.05157700
C	3.87324700	1.05578300	0.02680900
C	4.67875500	1.45514200	-1.05419200
H	4.21643300	1.94243500	-1.90841900
C	6.05313300	1.21869100	-1.04686900
H	6.65654000	1.52437000	-1.89778400
C	6.65122800	0.59522900	0.04951100
H	7.72277800	0.41406100	0.05831900
C	5.86479500	0.21050200	1.13694000
H	6.32262000	-0.26874500	1.99823500
C	4.48981400	0.44041400	1.12737700
H	3.88460800	0.14828900	1.97922200
C	1.16947000	-0.88198900	-0.01506300
C	-0.09898900	-1.40693200	-0.03660300
C	-0.56040800	-2.80515600	-0.08383200
C	0.09278600	-4.03453200	-0.17954000
H	1.17238300	-4.09684600	-0.22731200
C	-0.66726500	-5.21065100	-0.22038800
H	-0.15770800	-6.16793300	-0.29280600
C	-2.06421400	-5.17123000	-0.17612700
H	-2.63381700	-6.09605500	-0.21249900
C	-2.73206600	-3.94712300	-0.09926500
H	-3.81717400	-3.90769500	-0.08526800

C	-1.98046300	-2.77074800	-0.05121500
C	-2.42820600	-1.37961000	-0.02406500
C	-1.30262900	-0.55995300	-0.02045700
C	2.36666700	-1.77631000	-0.02003700
C	3.11227500	-1.97123000	-1.19009700
H	2.82840300	-1.44530400	-2.09720800
C	4.20846200	-2.83429900	-1.19701800
H	4.77601600	-2.97619400	-2.11284100
C	4.57544600	-3.51314800	-0.03362800
H	5.42979000	-4.18481600	-0.03992400
C	3.83891900	-3.32508800	1.13770400
H	4.11620500	-3.85152400	2.04741900
C	2.74146200	-2.46405700	1.14330300
H	2.16077700	-2.32686600	2.05161200
C	-3.87325800	-1.05579800	-0.02681500
C	-4.67874300	-1.45513200	1.05421300
H	-4.21640100	-1.94238900	1.90844900
C	-6.05312400	-1.21869800	1.04690500
H	-6.65651200	-1.52435500	1.89784200
C	-6.65124600	-0.59528300	-0.04948700
H	-7.72279900	-0.41413000	-0.05828200
C	-5.86483600	-0.21058800	-1.13694400
H	-6.32268300	0.26862000	-1.99824900
C	-4.48985200	-0.44048100	-1.12739500
H	-3.88466600	-0.14838400	-1.97926400

Anion **(TAInF1)**$^{\cdot -}$

Sum of electronic and zero-point Energies=	-1693.041953
Sum of electronic and thermal Energies=	-1693.009097
Sum of electronic and thermal Enthalpies=	-1693.008152
Sum of electronic and thermal Free Energies=	-1693.108157

C	-1.15470500	0.87462400	0.02060300
C	0.13857900	1.39928900	0.03049100
C	0.60927900	2.78260700	0.07149500
C	-0.03420700	4.02343500	0.18362300
H	-1.11309200	4.08601500	0.25354000

C	0.71694200	5.19953300	0.21826300
H	0.20722200	6.15727200	0.30223000
C	2.12033300	5.15615900	0.15615900
H	2.69265500	6.08178600	0.19027300
C	2.78417500	3.93792800	0.06817400
H	3.87047100	3.90514600	0.04819700
C	2.04250500	2.74176600	0.02241500
C	2.48454600	1.37094900	0.00517800
C	1.32182300	0.54380600	0.01239000
C	-2.33248400	1.79430900	0.04641500
C	-3.09640600	1.95830600	1.21052100
H	-2.83387200	1.38706800	2.09641200
C	-4.18016100	2.83674000	1.23984000
H	-4.75983700	2.94736600	2.15350300
C	-4.52225400	3.56990300	0.10216500
H	-5.36768400	4.25394300	0.12450100
C	-3.77096800	3.41641500	-1.06509600
H	-4.02711400	3.98373600	-1.95747500
C	-2.68783700	2.53786500	-1.08997500
H	-2.09486100	2.42829000	-1.99414800
C	3.92004100	1.03159900	0.03872500
C	4.78859000	1.52197700	-0.95817300
H	4.36718900	2.09514400	-1.77978000
C	6.16067900	1.27477800	-0.91704600
H	6.80101400	1.66232200	-1.70736600
C	6.71052700	0.52626300	0.12542400
H	7.77952000	0.32733700	0.15777000
C	5.86873900	0.03762900	1.12780300
H	6.28173400	-0.54203500	1.95071500
C	4.49966800	0.29414600	1.08921400
H	3.85977200	-0.07371300	1.88419500
C	1.15469500	-0.87461600	-0.02063700
C	-0.13858900	-1.39928300	-0.03052400
C	-0.60928400	-2.78260400	-0.07151100
C	0.03420400	-4.02343300	-0.18362600
H	1.11308800	-4.08601200	-0.25355000
C	-0.71694200	-5.19953400	-0.21824600
H	-0.20722000	-6.15727200	-0.30220400

C	-2.12033200	-5.15616200	-0.15613300
H	-2.69265300	-6.08179200	-0.19023100
C	-2.78417700	-3.93793200	-0.06816100
H	-3.87047200	-3.90515200	-0.04818100
C	-2.04251000	-2.74176600	-0.02242300
C	-2.48455700	-1.37095100	-0.00521200
C	-1.32183600	-0.54380000	-0.01243300
C	2.33248800	-1.79428500	-0.04641300
C	3.09640500	-1.95832400	-1.21051600
H	2.83385000	-1.38714200	-2.09643600
C	4.18018400	-2.83673200	-1.23979500
H	4.75985400	-2.94739400	-2.15345600
C	4.52230900	-3.56981900	-0.10208000
H	5.36775800	-4.25383500	-0.12438500
C	3.77103300	-3.41628000	1.06518100
H	4.02720600	-3.98353800	1.95759200
C	2.68787700	-2.53776000	1.09001900
H	2.09491000	-2.42814400	1.99419300
C	-3.92005700	-1.03162100	-0.03875900
C	-4.78858000	-1.52194200	0.95819000
H	-4.36715300	-2.09503500	1.77983600
C	-6.16067400	-1.27477300	0.91706900
H	-6.80098700	-1.66226700	1.70743100
C	-6.71055600	-0.52635200	-0.12545000
H	-7.77955400	-0.32745000	-0.15779300
C	-5.86879600	-0.03778400	-1.12788500
H	-6.28181700	0.54180300	-1.95083800
C	-4.49972000	-0.29427000	-1.08930000
H	-3.85984700	0.07353000	-1.88432600

Compound **TAInF2**

Sum of electronic and zero-point Energies=	-1771.562688
Sum of electronic and thermal Energies=	-1771.526020
Sum of electronic and thermal Enthalpies=	-1771.525076
Sum of electronic and thermal Free Energies=	-1771.635020

C	-2.44480600	-1.35150000	-0.01559100

C	-1.30922800	-0.54502600	-0.01621600
C	-1.15916500	0.89516000	0.01725500
C	0.11549400	1.40559300	0.03407300
C	0.59315200	2.79851300	0.07738600
C	-0.04554700	4.03551400	0.17363300
H	-1.12415100	4.11015600	0.22564900
C	0.72785900	5.20296600	0.20991500
H	0.22946000	6.16611500	0.28268600
C	2.12413200	5.14747300	0.16104700
H	2.70442500	6.06580100	0.19409600
C	2.77758100	3.91564900	0.08419200
H	3.86212500	3.86359400	0.06767600
C	2.01261700	2.74772300	0.04016300
C	2.44482000	1.35152500	0.01554000
C	1.30924400	0.54504300	0.01609400
C	1.15917900	-0.89514500	-0.01740900
C	-0.11548000	-1.40557700	-0.03422500
C	-0.59314500	-2.79849400	-0.07752400
C	0.04554700	-4.03549600	-0.17381100
H	1.12414900	-4.11013500	-0.22589000
C	-0.72786200	-5.20294600	-0.21005000
H	-0.22947000	-6.16609700	-0.28285300
C	-2.12413300	-5.14745000	-0.16109300
H	-2.70442700	-6.06578000	-0.19410700
C	-2.77757600	-3.91562700	-0.08419600
H	-3.86211900	-3.86356800	-0.06761500
C	-2.01260700	-2.74770000	-0.04021800
C	-3.88451100	-1.00931800	-0.02019200
C	-4.70396500	-1.40370100	1.05025300
H	-4.25833700	-1.90667600	1.90435800
C	-6.07409500	-1.14644100	1.03706100
H	-6.68258600	-1.45320400	1.88520300
C	-6.68003000	-0.50406500	-0.04905500
C	-5.86480300	-0.13372800	-1.12729200
H	-6.31041100	0.35357300	-1.99194400
C	-4.49474200	-0.37986000	-1.11645700
H	-3.88835400	-0.09243800	-1.96915600
C	-8.16013700	-0.20179500	-0.05504100

H	-8.59905000	-0.36149200	-1.04645000
H	-8.35373600	0.84434800	0.21800500
H	-8.70120700	-0.83107800	0.65928100
C	-2.34559700	1.80394900	0.02874100
C	-3.08138700	2.00808600	1.20344800
H	-2.79911200	1.47747500	2.10831100
C	-4.16540400	2.88632000	1.21796400
H	-4.72466100	3.03579400	2.13775800
C	-4.52994600	3.57160800	0.05752600
H	-5.37391400	4.25629000	0.06991300
C	-3.80349300	3.37411300	-1.11854500
H	-4.07885600	3.90533900	-2.02607900
C	-2.71838500	2.49768000	-1.13166200
H	-2.14523900	2.35341300	-2.04365000
C	3.88452200	1.00934600	0.02026100
C	4.70410900	1.40384600	-1.05001900
H	4.25861300	1.90693300	-1.90412600
C	6.07424800	1.14656900	-1.03668400
H	6.68283200	1.45344800	-1.88471700
C	6.68003100	0.50405600	0.04941600
C	5.86466100	0.13362600	1.12753400
H	6.31017500	-0.35374800	1.99219200
C	4.49461900	0.37977400	1.11655600
H	3.88810900	0.09230200	1.96915100
C	8.16011100	0.20166500	0.05553400
H	8.70134900	0.83110000	-0.65852300
H	8.35366100	-0.84441700	-0.21780600
H	8.59888300	0.36102400	1.04705500
C	2.34559900	-1.80394900	-0.02890300
C	3.08142200	-2.00803900	-1.20359800
H	2.79918600	-1.47737500	-2.10844300
C	4.16542800	-2.88628700	-1.21812500
H	4.72471000	-3.03572200	-2.13791000
C	4.52992500	-3.57163800	-0.05771100
H	5.37388500	-4.25633000	-0.07010700
C	3.80343500	-3.37419900	1.11834500
H	4.07876000	-3.90547600	2.02586100
C	2.71833600	-2.49775500	1.13147200

H	2.14516100	-2.35353000	2.04344800

Anion **(TAInF2)**$^{\cdot -}$

Sum of electronic and zero-point Energies=	-1771.621990
Sum of electronic and thermal Energies=	-1771.585287
Sum of electronic and thermal Enthalpies=	-1771.584343
Sum of electronic and thermal Free Energies=	-1771.694400

C	-2.49364600	1.35404700	-0.00854700
C	-1.32531300	0.53508200	0.00457600
C	-1.14877900	-0.88224800	-0.02615400
C	0.14792000	-1.39853300	-0.02831700
C	0.62836500	-2.77855600	-0.06550500
C	-0.00590500	-4.02396700	-0.17904700
H	-1.08402600	-4.09406400	-0.25381500
C	0.75354100	-5.19489500	-0.20874400
H	0.25088500	-6.15628500	-0.29375100
C	2.15635900	-5.14165700	-0.14018700
H	2.73522300	-6.06336900	-0.17044000
C	2.81129000	-3.91873000	-0.05055500
H	3.89725300	-3.87819900	-0.02544000
C	2.06117300	-2.72764900	-0.00979700
C	2.49364700	-1.35402600	0.00851300
C	1.32531200	-0.53505300	-0.00464000
C	1.14878000	0.88227400	0.02610000
C	-0.14792000	1.39856500	0.02826800
C	-0.62837000	2.77858600	0.06548900
C	0.00588200	4.02400300	0.17905000
H	1.08400200	4.09411800	0.25381800
C	-0.75357600	5.19492300	0.20878000
H	-0.25092700	6.15631500	0.29380300
C	-2.15639400	5.14167500	0.14024400
H	-2.73526500	6.06338100	0.17052200
C	-2.81131300	3.91874200	0.05060000
H	-3.89727600	3.87819400	0.02549700
C	-2.06118300	2.72767000	0.00980900
C	-3.92608600	1.00248800	0.01948600

C	-4.79962800	1.48242000	-0.97562500
H	-4.38779400	2.06325600	-1.79675200
C	-6.16906200	1.22131900	-0.93519400
H	-6.80981100	1.60635100	-1.72775000
C	-6.73340900	0.46621400	0.09890500
C	-5.87277800	-0.00315600	1.10100400
H	-6.28149800	-0.58224100	1.92796300
C	-4.50722300	0.26333000	1.06780800
H	-3.87139600	-0.09604100	1.86999300
C	-8.21045600	0.14619500	0.12561000
H	-8.61344400	0.18378700	1.14532800
H	-8.41551200	-0.86250600	-0.26116800
H	-8.78485300	0.85063600	-0.48717900
C	-2.32065900	-1.80935900	-0.05883800
C	-3.07582600	-1.97896100	-1.22788600
H	-2.81098200	-1.40654100	-2.11231000
C	-4.15359500	-2.86450500	-1.26401300
H	-4.72590800	-2.97985700	-2.18178200
C	-4.49857600	-3.59933000	-0.12820700
H	-5.33882700	-4.28958400	-0.15594400
C	-3.75610500	-3.44024500	1.04395800
H	-4.01445300	-4.00877800	1.93492900
C	-2.67894700	-2.55458500	1.07556200
H	-2.09279500	-2.44068300	1.98363300
C	3.92608000	-1.00247900	-0.01952900
C	4.79963600	-1.48246000	0.97555200
H	4.38780500	-2.06330200	1.79667500
C	6.16907200	-1.22138700	0.93510700
H	6.80982100	-1.60644800	1.72765000
C	6.73342000	-0.46625600	-0.09897400
C	5.87277500	0.00318900	-1.10102500
H	6.28148200	0.58233200	-1.92795000
C	4.50721500	-0.26327300	-1.06781900
H	3.87138600	0.09615600	-1.86997500
C	8.21049400	-0.14637500	-0.12576600
H	8.78479800	-0.85054900	0.48742100
H	8.41562500	0.86251600	0.26046900
H	8.61353600	-0.18456500	-1.14544600

C	2.32066000	1.80938500	0.05884800
C	3.07581500	1.97889600	1.22791800
H	2.81095600	1.40641100	2.11229500
C	4.15358900	2.86443100	1.26412300
H	4.72589000	2.97971500	2.18190700
C	4.49859100	3.59933100	0.12837100
H	5.33884800	4.28957600	0.15616700
C	3.75614000	3.44032800	-1.04381600
H	4.01450800	4.00891800	-1.93474600
C	2.67897600	2.55467900	-1.07549800
H	2.09284100	2.44083900	-1.98358800

Compound **TAInF3**

Sum of electronic and zero-point Energies=	-2334.559631
Sum of electronic and thermal Energies=	-2334.527391
Sum of electronic and thermal Enthalpies=	-2334.526446
Sum of electronic and thermal Free Energies=	-2334.625740

S	5.00522700	1.36683600	-1.09292600
C	1.13293100	-0.92704500	0.01633300
C	1.32191800	0.50658100	0.07294700
C	0.15510700	1.39967200	0.05853900
C	0.66749300	2.77873900	0.13337700
C	0.05426700	4.02905000	0.22290600
H	-1.02332000	4.12776400	0.23822300
C	0.85224600	5.17736400	0.30264000
H	0.37403100	6.15104700	0.36938400
C	2.24716100	5.08852600	0.30639000
H	2.84786400	5.99156700	0.37412500
C	2.87429400	3.84258200	0.23732100
H	3.95683300	3.76847900	0.26293500
C	2.08505300	2.69384000	0.14676100
C	2.47999900	1.28461000	0.12299300
C	3.88619500	0.88129800	0.17846700
C	4.56374000	0.19460800	1.15725800
H	4.07243600	-0.18350900	2.04524600

C	5.95595600	0.04105300	0.89522200
H	6.63896100	-0.47657700	1.56012100
C	6.34138900	0.61667300	-0.28379400
H	7.32737700	0.64043300	-0.72881700
C	2.28896800	-1.87369700	0.04386000
C	3.05124400	-2.10855700	-1.10791800
H	2.81387200	-1.57458600	-2.02362100
C	4.10612500	-3.02160200	-1.08516800
H	4.68807200	-3.19367900	-1.98667200
C	4.41258300	-3.71224200	0.08893000
H	5.23383500	-4.42386700	0.10525600
C	3.65705700	-3.48565900	1.24135200
H	3.88627600	-4.02201400	2.15865400
C	2.60138800	-2.57387800	1.21783000
H	2.00524900	-2.40679500	2.11107500
S	-5.00521400	-1.36684900	1.09295600
C	-1.13293700	0.92704400	-0.01635900
C	-1.32192600	-0.50658300	-0.07297600
C	-0.15511400	-1.39967500	-0.05856500
C	-0.66750100	-2.77874300	-0.13340600
C	-0.05427700	-4.02905500	-0.22294900
H	1.02330900	-4.12777100	-0.23828200
C	-0.85225800	-5.17736800	-0.30267500
H	-0.37404500	-6.15105200	-0.36942800
C	-2.24717300	-5.08853100	-0.30640400
H	-2.84787800	-5.99157000	-0.37413200
C	-2.87430400	-3.84258600	-0.23732400
H	-3.95684300	-3.76848100	-0.26292600
C	-2.08506100	-2.69384400	-0.14677400
C	-2.48000700	-1.28461500	-0.12300600
C	-3.88620700	-0.88131300	-0.17846100
C	-4.56377800	-0.19465100	-1.15725400
H	-4.07249500	0.18345100	-2.04525900
C	-5.95599100	-0.04110800	-0.89519700
H	-6.63901400	0.47650100	-1.56009400
C	-6.34139800	-0.61671200	0.28383600
H	-7.32737800	-0.64047600	0.72887600
C	-2.28896500	1.87370700	-0.04387100

C	-3.05125900	2.10853100	1.10790200
H	-2.81391700	1.57451400	2.02358600
C	-4.10612400	3.02159600	1.08517200
H	-4.68808700	3.19364200	1.98667000
C	-4.41254000	3.71230000	-0.08890000
H	-5.23377600	4.42394200	-0.10521000
C	-3.65698900	3.48576100	-1.24131400
H	-3.88617300	4.02216900	-2.15859500
C	-2.60134100	2.57395700	-1.21781300
H	-2.00518100	2.40690800	-2.11105000

Anion **(TAInF3)**$^{\cdot -}$

Sum of electronic and zero-point Energies=	-2334.625831
Sum of electronic and thermal Energies=	-2334.593424
Sum of electronic and thermal Enthalpies=	-2334.592479
Sum of electronic and thermal Free Energies=	-2334.692380

S	5.07092700	1.35580100	-1.07629600
C	1.12233800	-0.91536600	0.01454300
C	1.33679300	0.49448700	0.06805500
C	0.18767700	1.39140500	0.05476900
C	0.70436200	2.75689300	0.13601000
C	0.09660300	4.01654900	0.23357600
H	-0.98184000	4.11355500	0.25119000
C	0.88458900	5.16557100	0.31974000
H	0.40404300	6.13915400	0.39220400
C	2.28647900	5.07507900	0.32255200
H	2.88726000	5.98008300	0.39488000
C	2.91330800	3.83592800	0.24769300
H	3.99740000	3.76690300	0.27261200
C	2.13432800	2.66841500	0.15281700
C	2.52837500	1.28089600	0.12684200
C	3.92569900	0.86596400	0.18956800
C	4.60284400	0.13499700	1.13844600
H	4.10475700	-0.26261800	2.01433900
C	5.99219800	-0.04146800	0.87147000

H	6.66199500	-0.59161500	1.52573600
C	6.39923700	0.56670500	-0.28391800
H	7.39520500	0.60706600	-0.70609900
C	2.26481200	-1.87861500	0.04264000
C	3.05546500	-2.10022300	-1.09340300
H	2.84323100	-1.54137000	-2.00031600
C	4.10420600	-3.02030800	-1.06797000
H	4.70715800	-3.17443700	-1.95992500
C	4.38175200	-3.73858600	0.09667300
H	5.19926300	-4.45588400	0.11661900
C	3.60178300	-3.52787900	1.23588400
H	3.80734800	-4.08364300	2.14840700
C	2.55394800	-2.60729500	1.20655200
H	1.93840600	-2.45247800	2.08876500
S	-5.07089400	-1.35583100	1.07637400
C	-1.12235300	0.91536000	-0.01460200
C	-1.33681200	-0.49449500	-0.06812200
C	-0.18769300	-1.39141600	-0.05483100
C	-0.70438100	-2.75690400	-0.13608600
C	-0.09663100	-4.01656300	-0.23369000
H	0.98181000	-4.11357600	-0.25134400
C	-0.88462300	-5.16558300	-0.31984000
H	-0.40408200	-6.13916500	-0.39233000
C	-2.28651200	-5.07508800	-0.32260100
H	-2.88729900	-5.98008900	-0.39491700
C	-2.91333400	-3.83593600	-0.24771100
H	-3.99742600	-3.76690600	-0.27259800
C	-2.13434700	-2.66842500	-0.15285200
C	-2.52839500	-1.28090900	-0.12686900
C	-3.92572800	-0.86599700	-0.18954700
C	-4.60293500	-0.13509200	-1.13842800
H	-4.10489800	0.26249200	-2.01436400
C	-5.99228000	0.04135200	-0.87139800
H	-6.66212000	0.59145500	-1.52565700
C	-6.39925500	-0.56678600	0.28403100
H	-7.39520400	-0.60715700	0.70625700
C	-2.26480400	1.87863600	-0.04266400
C	-3.05549700	2.10016700	1.09336500

H	-2.84332900	1.54121400	2.00023200
C	-4.10419700	3.02030200	1.06797600
H	-4.70718600	3.17436400	1.95991800
C	-4.38164800	3.73871900	-0.09660200
H	-5.19912200	4.45606000	-0.11651300
C	-3.60162400	3.52810500	-1.23579400
H	-3.80711100	4.08398400	-2.14826400
C	-2.55383700	2.60746600	-1.20650800
H	-1.93825100	2.45272200	-2.08870300

1. *Gaussian 09; Revision A.2*; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R.; Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. J. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N.; Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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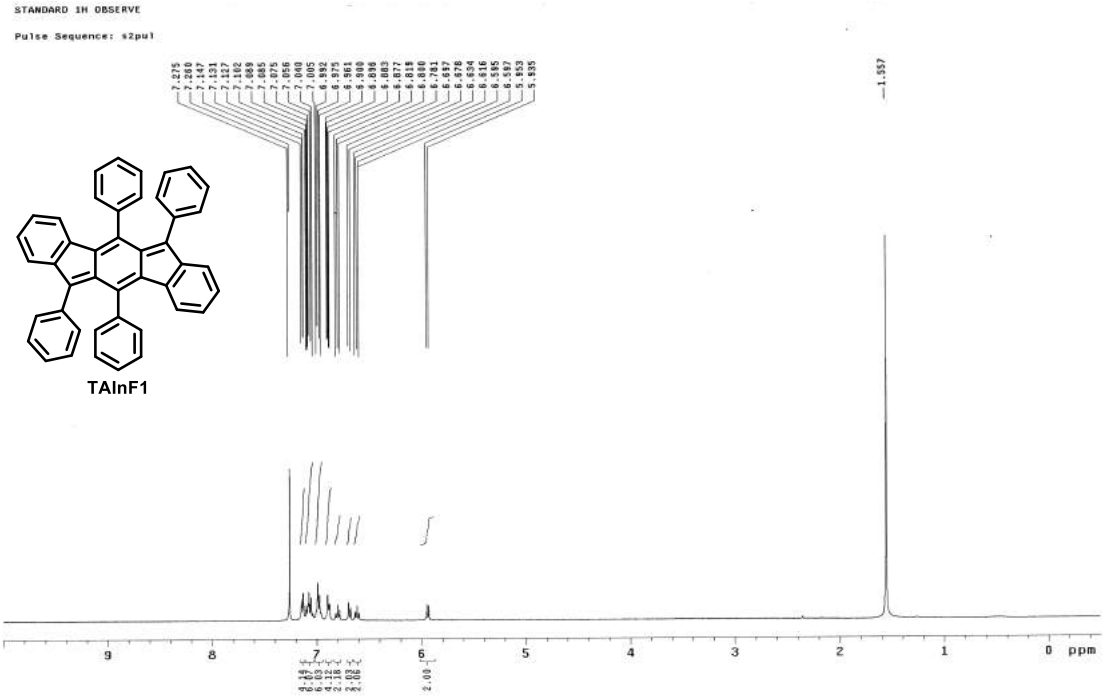
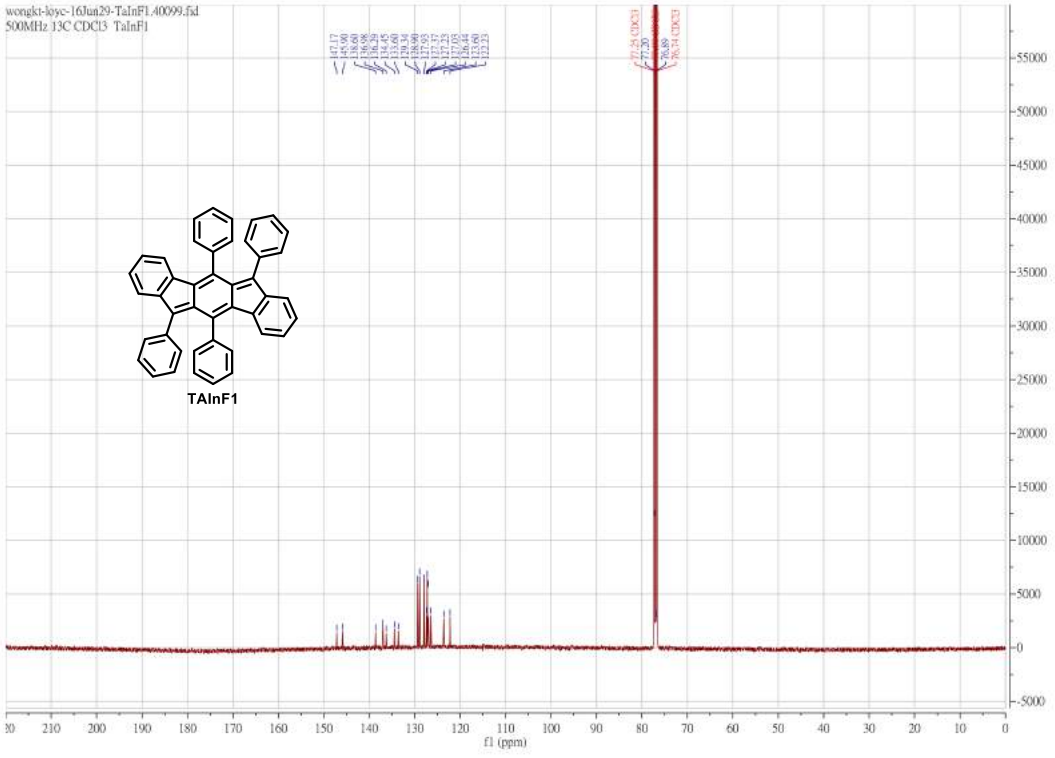
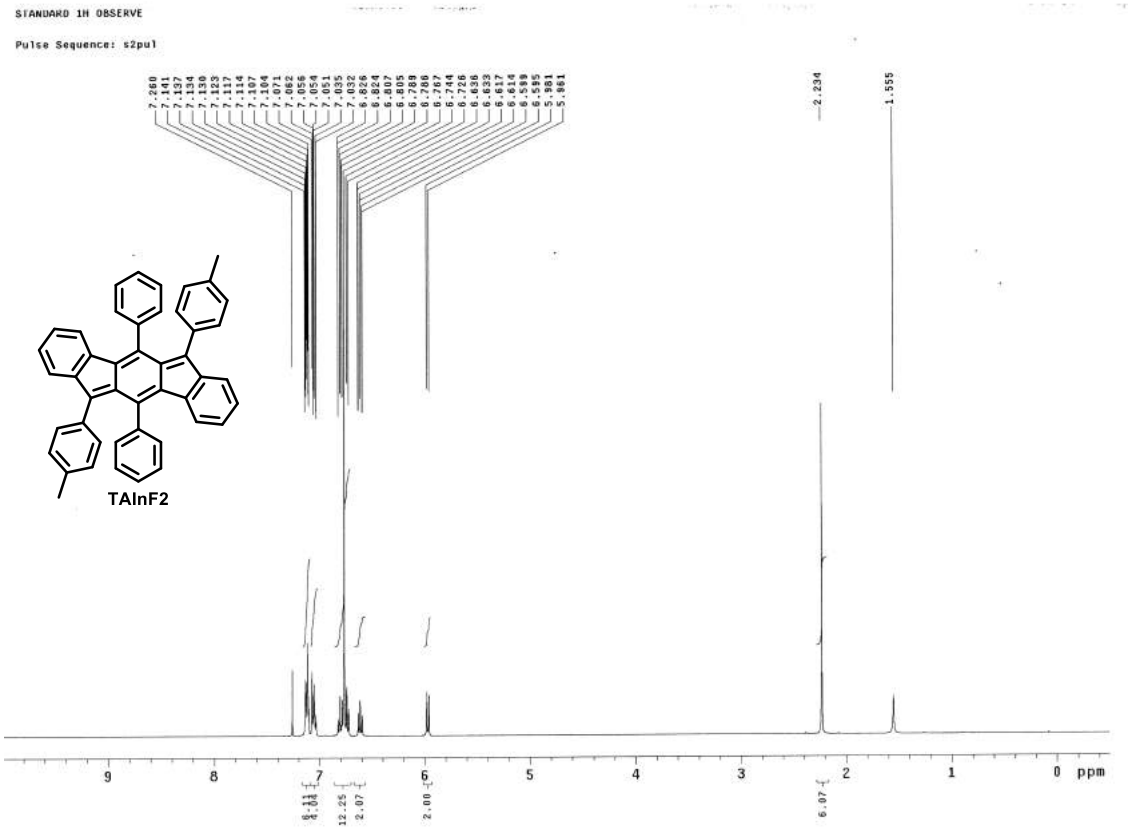
NMR spectra of **TAInF1**, **TAInF2** and **TAInF3**



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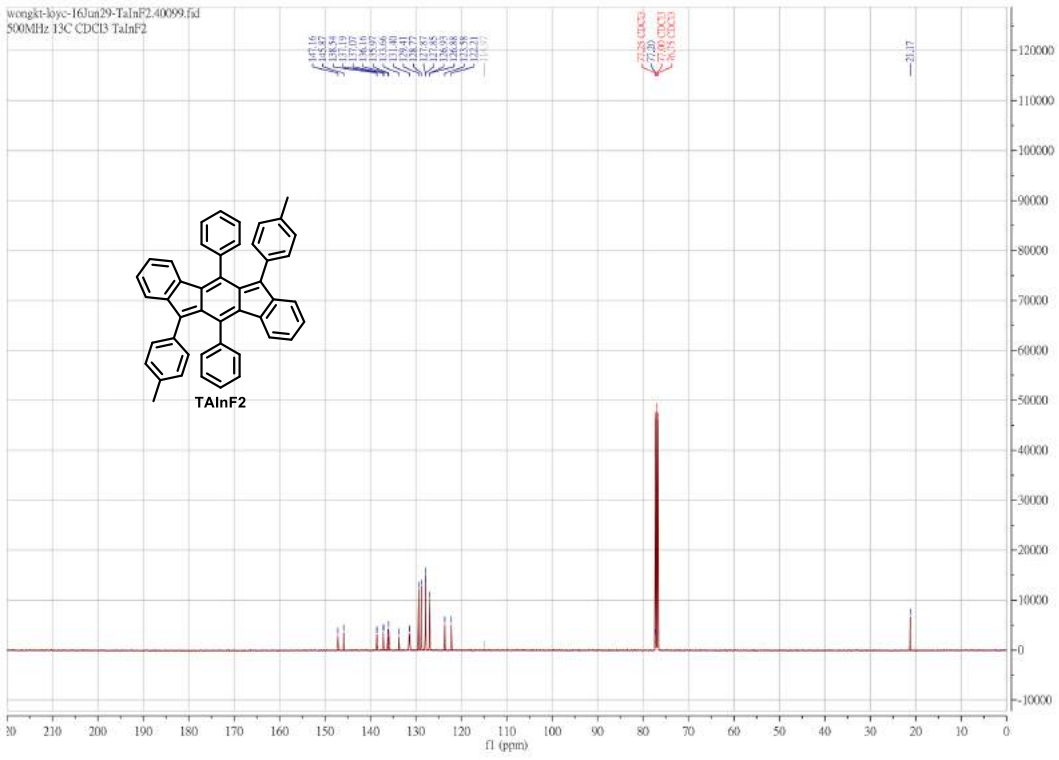
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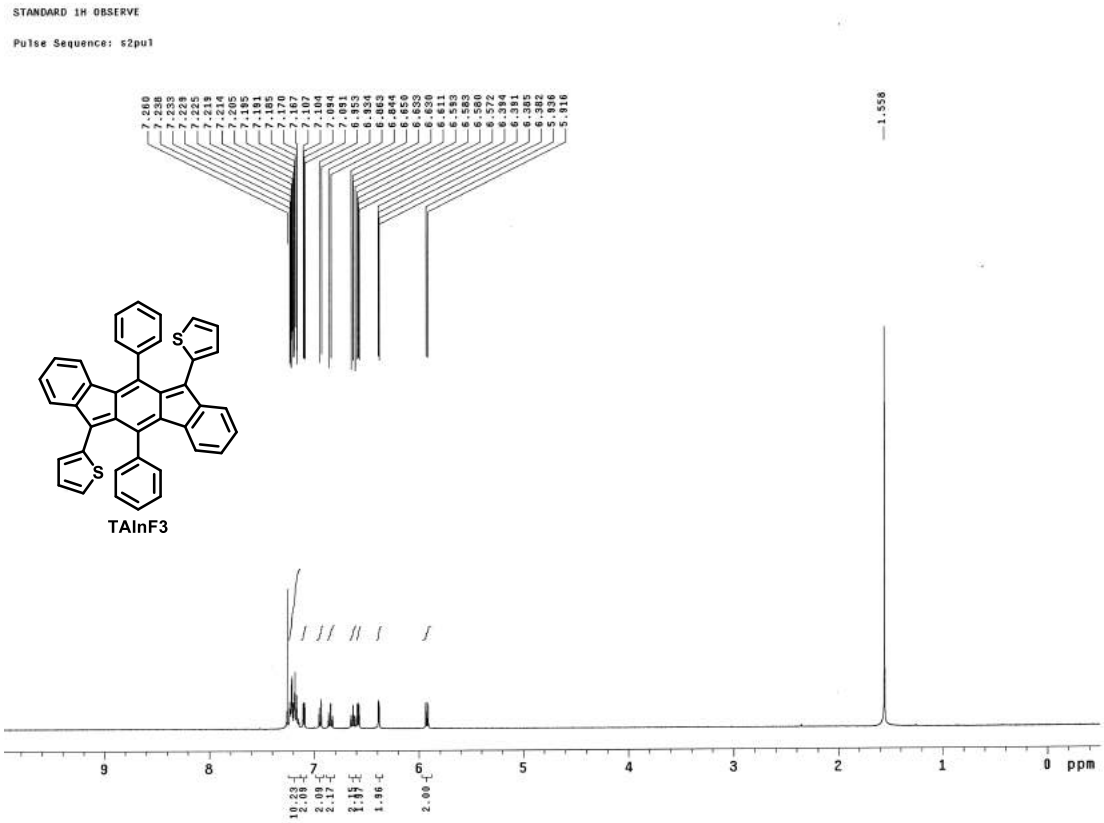
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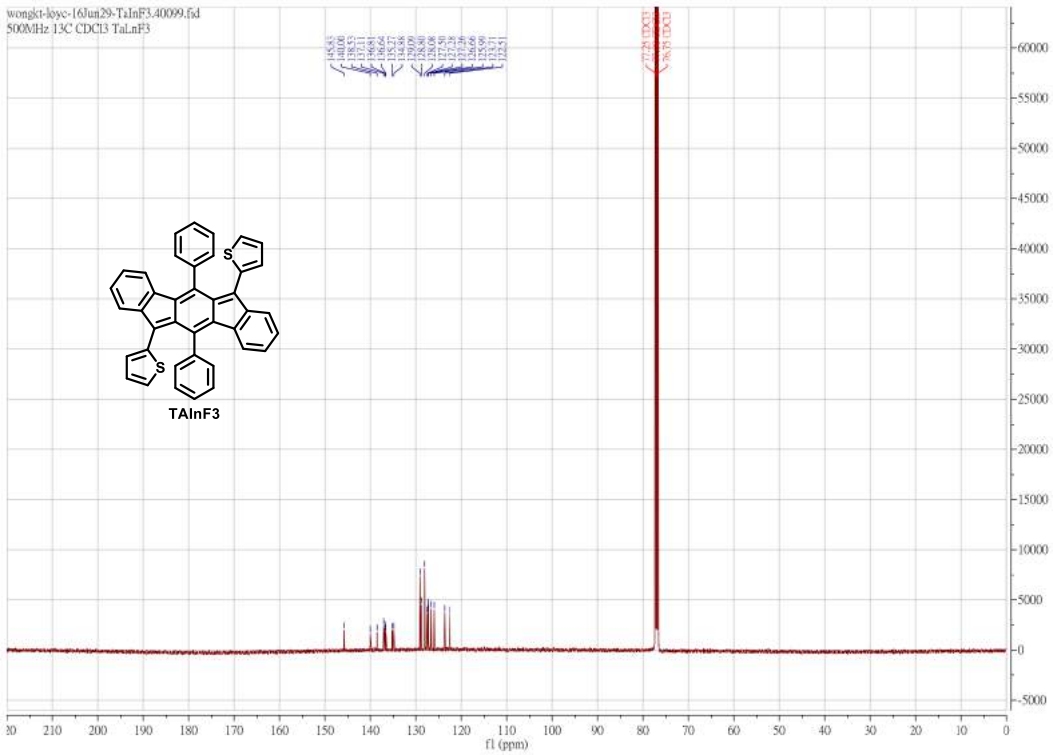
ppm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