Supporting Information

Halogen Bonding vs π-Stacking Interactions in New Bis(acenaphthylene)dione Semiconductors

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Contents

I. Measurements and Instruments

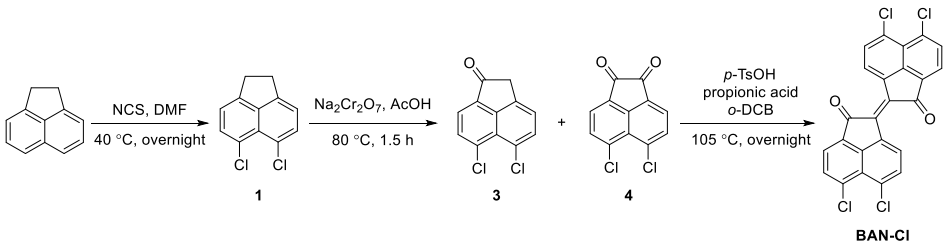
The NMR spectra were measured by Bruker AVIIIHD 500 MHz or Varian Mercury 400 MHz NMR spectrometer for ^{1}H and ^{13}C NMR, and by Varian VNMRS spectrometer for solid-state NMR. The mass spectra were measured by Bruker Maxis with atmospheric pressure ionization (API). The FTIR spectra were measured by FT-IR infrared spectrometer Alpha II from Bruker with powder samples. The UV-Vis absorption spectra were recorded on a JASCO V-670 spectrophotometer. Solutions were prepared in DMF and the spectra were recorded in 10 mm path length quarts cells. The solid-state absorption spectra were recorded on the same instrument using thin films, vapor-deposited on glass substrates in vacuum with a thickness of about 40 nm. The emission spectra in solution (DMF) were measured on Varian Cary Eclipse fluorescence spectrophotometer. Solid-state emission spectra were recorded using vapor-deposited thin-films on glass on a film holder on Fluorolog-3 spectrometer from Horiba Scientific.

II. Device Fabrication

Thin-film FETs were fabricated on prepatterned bottom-contact bottom-gate configurations (with symmetric Au electrodes as the drain and source with different channel lengths of 2.5, 5, 10, and 20 μm). The performance of the resulting OFETs was measured in a vacuum and ambient atmosphere using a Keithley 4200-SCS semiconductor parameter analyzer. Thin film of BAN derivatives was grown by vacuum deposition (~10^{-6} mbar, deposition rate 0.1–0.3 Å/s) on dodecyltrichlorosilane (DTS) surface treated SiO_2/Si wafers. SiO_2 was thermally grown (200 nm thick, C = 1.8×10^{-8} F/cm^2) on heavily n-doped (Sb) Si ($\rho \approx 0.01$ Ohm cm). For DTS functionalization, samples were washed with acetone and 2-propanol and cleaned in PDC-32G plasma cleaner. The sample was then heated in 5 mM solution of DTS in toluene at 60 °C for 40 min. Subsequently, they were rinsed with toluene and dried at 60 °C in air for 10 min prior to thin-film deposition.

III. Synthesis and Characterization

Acenaphthene, *N*-chlorosuccinimide (NCS), *N*-bromosuccinimide (NBS), *p*-toluenesulfonic acid (*p*-TsOH), propionic acid, *o*-dichlorobenzene (*o*-DCB) were purchased from Sigma Aldrich. Hydrochloric acid (35%), glacial acetic acid (AcOH), hexanes, ethyl acetate (EtOAc), dichloromethane (DCM), and *N*,*N*-dimethylformamide (DMF) were purchased from Fisher Scientific. Sodium dichromate ($Na_2Cr_2O_7$) was purchased from Anachemia Chemicals. All chemicals were used as received.



5,6-Dichloro-1,2-dihydroacenaphthylene (**1**):

To the solution of acenaphthene (8.00 g, 51.9 mmol) in 70 mL DMF, NCS (15.25 g, 114.2 mmol) was added in portion, stirring in an ice bath. The reaction mixture was heated to 40 °C overnight. The reaction was quenched by adding $Na_2S_2O_3$ aqueous solution in an ice bath. The mixture was extracted by EtOAc and water. The organic layer was dried over $MgSO_4$ and concentrated under reduces pressure. The residue was placed in the cold room forming precipitate. The precipitate was purified by recrystallizing from EtOH. Yield: 2.05 g (18%).

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 7.51 (d, 2H, *J* = 7.4 Hz, $CH_{arom.}$), 7.17 (d, 2H, *J* = 7.4 Hz, $CH_{arom.}$), 3.35 (s, 4H, CH_2) ppm.

^{13}C-NMR (125 MHz, $CDCl_3$): δ = 146.17, 142.00, 131.30, 126.31, 125.57, 120.26, 30.00 ppm.

HRMS (APCI): *m/z* [M^+] 222.0001 (Cal. 221.9998).

5,6-Dichloroacenaphthylen-1(2*H*)-one (**3**) and 5,6-dichloroacenaphthylene-1,2-dione (**4**):

A solution of $Na_2Cr_2O_7$ (590 mg, 2.25 mmol) in AcOH (7 mL) was added dropwise to a suspension of **1** (500 mg, 2.25 mmol) in AOH (2 mL), stirring at room temperature for 15 min. The reaction mixture was heated to 80 °C for 1.5 h. The reaction mixture was poured into the ice-water with conc. HCl. The orange precipitate (489 mg, 89%) was collected by filtration and dried in vacuum. Because of poor solubility, it's hard to well purify **3** and **4** by silica chromatography. The ratio of **3** and **4** in the crude product was optimized to 1:1.07 (based on ^{1}H-NMR) and used directly for synthesis of **BAN-Cl**. For the purpose of analysis, **3** and **4** were separated by silica chromatography (DCM: EtOAc 20:1 v/v).

^{1}H-NMR (400 MHz, $CDCl_3$) for **3**: δ = 7.87 (d, 1H, *J* = 7.6 Hz, $CH_{arom.}$), 7.81 (d, 1H, *J* = 7.6 Hz, $CH_{arom.}$), 7.70 (d, 1H, *J* = 7.4 Hz, $CH_{arom.}$), 7.40 (d, 1H, *J* = 7.4 Hz, $CH_{arom.}$), 3.80 (s, 2H, CH_2) ppm.

HRMS (APCI) for **3**: *m/z* [M^-] 234.9719 (Cal. 234.9723).

^{1}H-NMR (400 MHz, $CDCl_3$) for **4**: δ = 8.04 (d, 2H, *J* = 7.5 Hz, $CH_{arom.}$), 7.94 (d, 2H, *J* = 7.9 Hz, $CH_{arom.}$) ppm.

HRMS (APCI) for **4**: *m/z* [M^-] 249.9592 (Cal. 249.9594).

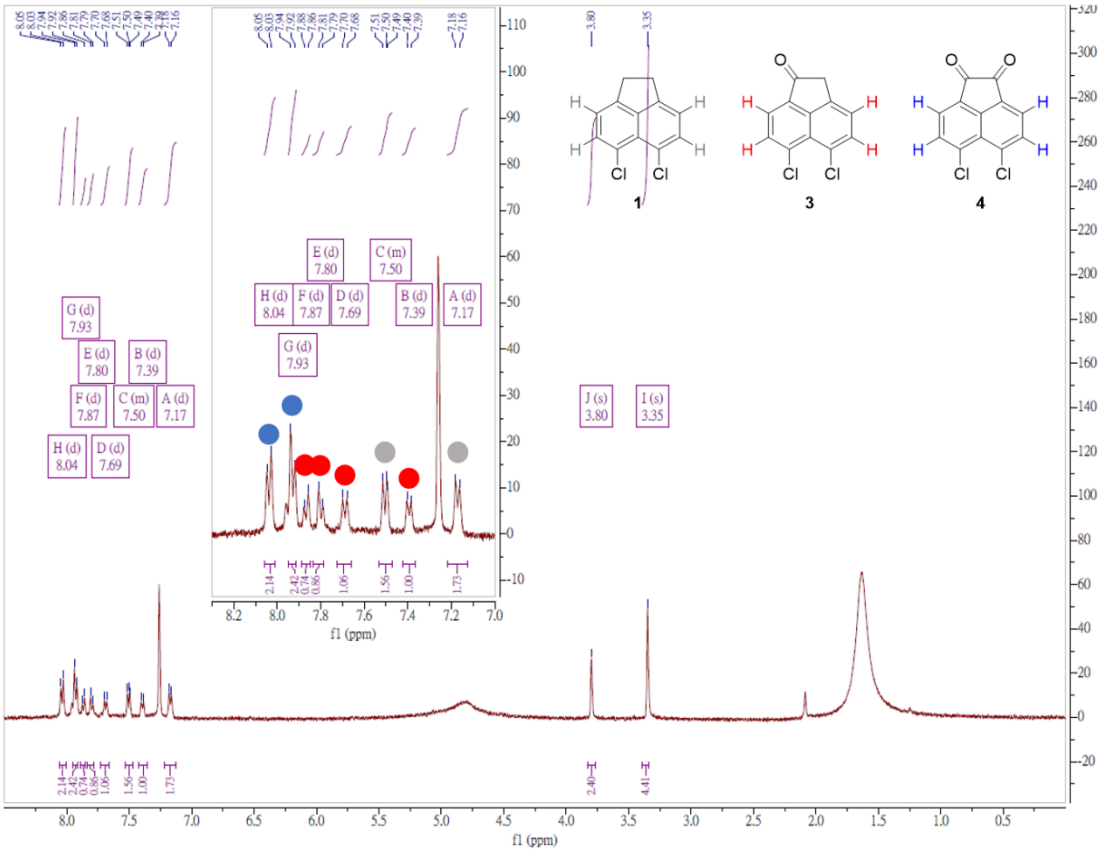


Figure S1. ^{1}H-NMR of 5,6-Dichloroacenaphthylen-1(2*H*)-one (**3**) and 5,6-dichloroacenaphthylene-1,2-dione (**4**) with a ratio of 1:1.07.

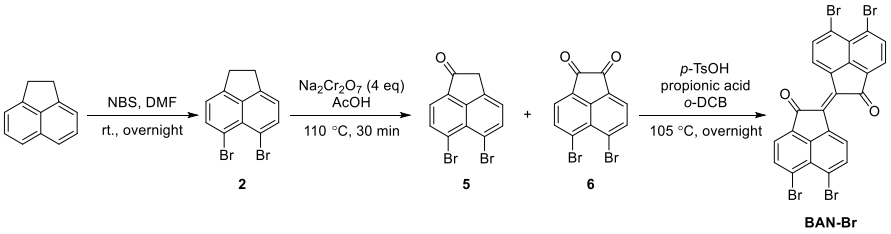
(*E*)-5,5',6,6'-Tetrachloro-2*H*,2'*H*-[1,1'-biacenaphthylenylidene]-2,2'-dione (**BAN-Cl**): Modified based on a literature procedure.[1] In a round-bottom flask, the crude product of **3** and **4** (1.90 g with **3**:**4** 1:1.07, 4.0 mmol for **3**) was placed with *p*-TsOH (2.28 g, 12.0 mmol), propionic acid (0.9 mL, 12.0 mmol), and *o*-DCB (50 mL). The reaction mixture was heated to 105 °C overnight. After cooling down to the room temperature, the reaction mixture was poured into methanol. The red precipitate (1.09 g) was collected by filtration, washed with acetone, DCM, and water, and dried in vacuum. Because of poor solubility, the product was purified by gradient sublimation at 280–310 °C under 10^{-5} mbar.

^{13}C CPMAS: 192.1, 141.3, 138.7, 135.1, 131.1, 129.0, 123.1, 122.0.

HRMS (APCI): *m/z* [M-H^{+}] 468.9360 (Cal.: 468.9351).

FT-IR (ATR): ν = 3135, 3066, 1699, 1563, 1414, 1353, 1330, 1248, 1220, 1030, 1008, 838, 753, 655.

Element analysis: calculated for $C_{24}H_8Cl_4O_2$: C 61.32, H 1.72, found: C 64.63, H 1.86.



5,6-Dibromo-1,2-dihydroacenaphthylene (**2**):

Modified based on a literature procedure.[2] To the solution of acenaphthene (12.00 g, 77.9 mmol) in DMF (90 mL), NBS (30.50 g, 171.3 mmol) was added in portions in an ice bath. The reaction mixture was allowed to warm to room temperature stirring overnight to afford a brown solution with yellow precipitate. The precipitate was collected by filtration and washed with EtOH. The precipitate was purified by recrystallizing from hot EtOH solution. Yield: 5.03 g (21%). NMR data were in accordance with those reported in the literature.[3]

^{1}H-NMR (500 MHz, $CDCl_3$): δ = 7.81 (d, 2H, *J* = 7.4 Hz, $CH_{arom.}$), 7.10 (dt, 2H, *J* = 7.5 Hz, $CH_{arom.}$), 3.32 (s, 4H, CH_2) ppm.

5,6-Dibromoacenaphthylen-1(2*H*)-one (**5**) and 5,6-dibromoacenaphthylene-1,2-dione (**6**):

Modified based on a literature procedure.[4] A solution of $Na_2Cr_2O_7$ (1.25 g, 4.8 mmol) in AcOH (12 mL) was added dropwise to the suspension of **2** (372 mg, 1.19 mmol) in AcOH (3 mL), stirring at room temperature for 15 min. The reaction mixture was heated to 110 °C for 30 min. The reaction was poured on the ice-water with conc. HCl. The orange precipitate (385 mg, 96%) was collected by filtration and dried in vacuum. Because of poor solubility, it is difficult to efficiently separate **5** and **6** by chromatography. Therefore, the ratio of **5** and **6** in the crude product was optimized to 1:3.5 (based on ^{1}H-NMR) and used directly for synthesis of **BAN-Br**. For the purpose of analysis, **5** and **6** were separated by silica chromatography (DCM: EtOAc 20:1 v/v). NMR data of **6** were in accordance with those reported in the literature.[4]

^{1}H-NMR (400 MHz, $CDCl_3$) for **5**: δ = 8.12 (d, 1H, *J* = 7.5 Hz, $CH_{arom.}$), 8.01 (d, 1H, *J* = 7.5 Hz, $CH_{arom.}$), 7.93 (d, 1H, *J* = 7.5 Hz, $CH_{arom.}$), 7.77 (d, 1H, *J* = 7.7 Hz, $CH_{arom.}$), 3.78 (s, 2H, CH_2) ppm.

HRMS for **5**: *m/z* [M^-] 322.8716 (Cal. 322.8713).

^{1}H-NMR (400 MHz, $CDCl_3$) for **6**: δ = 8.26 (d, 2H, *J* = 7.5 Hz, $CH_{arom.}$), 7.93 (d, 2H, *J* = 7.5 Hz, $CH_{arom.}$) ppm.

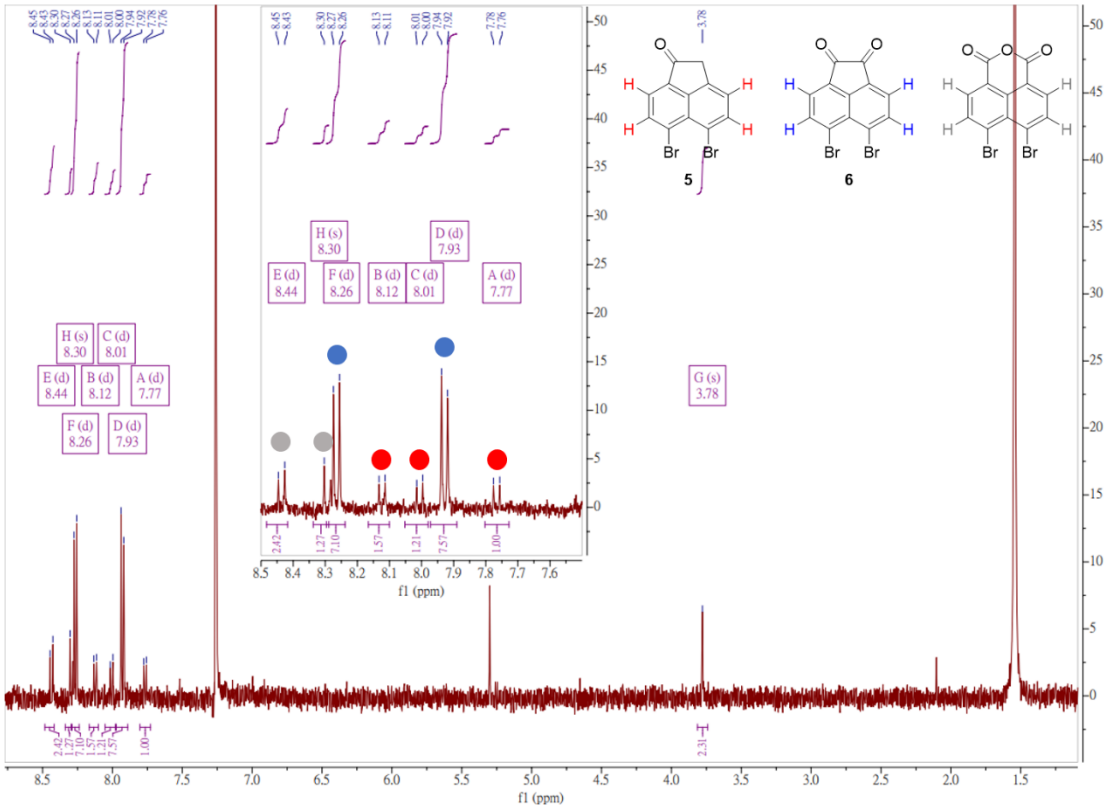


Figure S2. ^{1}H-NMR of 5,6-Dibromoacenaphthylen-1(2*H*)-one (**5**) and 5,6-Dibromoacenaphthylene-1,2-dione (**6**) with a ratio of 1:3.5.

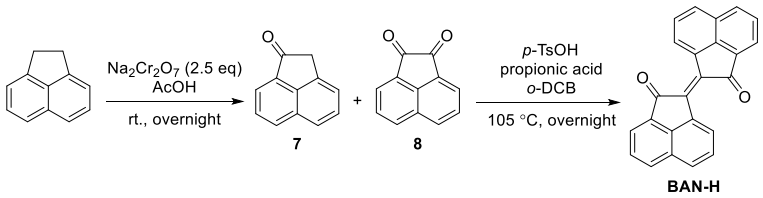
(*E*)-5,5',6,6'-Tetrabromo-2*H*,2'*H*-[1,1'-biacenaphthylenylidene]-2,2'-dione (**BAN-Br**): Modified based on a literature procedure.[1] In a round-bottom flask, the crude product of **5** and **6** (1.32 g with **5**:**6** 1:3.55, 0.9 mmol for **5**) was placed with *p*-TsOH (514 mg, 2.7 mmol), propionic acid (0.2 mL, 2.7 mmol), and *o*-DCB (20 mL). The reaction mixture was heated to 105 °C overnight. After cooling down to the room temperature, the reaction mixture was poured into methanol. The red precipitate (420 mg) was collected by filtration, washed with acetone, DCM, and water, and dried in vacuum. Because of poor solubility, the product was purified by gradient sublimation at 280-310 °C under 10^{-5} mbar.

^{13}C CPMAS: 191.5, 141.2, 135.3, 131.9, 131.0, 129.5, 128.0.

HRMS (APCI): *m/z* [M^{+}] 643.7248 (Cal. 643.7263).

FT-IR (ATR): ν = 3135, 3074, 1697, 1552, 1403, 1323, 1242, 1211, 1036, 1018, 838, 800, 753, 653.

Element analysis: calculated for $C_{24}H_8Br_4O_2$: C 44.49, H 1.24, found: C 44.73, H 1.02.



Acenaphthylen-1(2*H*)-one (**7**) and acenaphthylene-1,2-dione (**8**):

A solution of $Na_2Cr_2O_7$ (851 mg, 3.25 mmol) in AcOH (18 mL) was added dropwise to the suspension of acenaphthene (200 mg, 1.30 mmol) in AcOH (2 mL). After stirring at room temperature overnight, the reaction mixture was poured on the ice-water with conc. HCl. The mixture was extracted with EtOAc. The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. The proposed molecules were separated and purified by silica chromatography (Hex:EtOAc 4:1 v/v). Yield: 69 mg (32%) for **7** and 39 mg (16%) for **8**. NMR data of **7** and **8** were in accordance with those reported in the literature.[5, 6]

^{1}H-NMR (500 MHz, $CDCl_3$) for **7**: δ = 8.10 (d, 1H, *J* = 8.1 Hz, $CH_{arom.}$), 7.97 (d, 1H, *J* = 7.0 Hz, $CH_{arom.}$), 7.83 (d, 1H, *J* = 8.4 Hz, $CH_{arom.}$), 7.72 (t, 1H, *J* = 7.6 Hz, $CH_{arom.}$), 7.61 (dd, 1H, *J* = 8.4, 6.8 Hz, $CH_{arom.}$), 7.48 (d, 1H, *J* = 6.9 Hz, $CH_{arom.}$), 3.83 (s, 2H, CH_2) ppm.

^{1}H-NMR (400 MHz, $CDCl_3$) for **8**: δ = 8.30 (d, 2H, *J* = 8.4 Hz, $CH_{arom.}$), 8.13 (d, 2H, *J* = 7.0 Hz, $CH_{arom.}$), 7.87 (t, 2H, *J* = 7.7 Hz, $CH_{arom.}$) ppm.

(*E*)-2*H*,2'*H*-[1,1'-biacenaphthylenylidene]-2,2'-dione (BAN-H):

Modified based on a literature procedure.[1] In a round-bottom flask, **7** (48 mg, 0.29 mmol) and **8** (63 mg, 0.35 mmol) were placed with *p*-TsOH (165 mg, 0.87 mmol), propionic acid (0.07 mL, 0.87 mmol), and *o*-DCB (1 mL). The reaction mixture was heated to 105 °C overnight. After cooling down to the room temperature, the reaction mixture was poured into methanol. The brown precipitate was filtered off, washed with methanol and water, and dried in vacuum. BAN-H was purified by silica chromatography (Hex:EtOAc 3:1 v/v) as orange powders. Yield: 27 mg (28%). NMR data of BAN-H was in accordance with those reported in the literature.[7]

^{1}H-NMR (400 MHz, $CDCl_3$) for BAN-H: δ = 9.48 (d, 1H, *J* = 7.5 Hz, $CH_{arom.}$), 8.16 (d, 1H, *J* = 8.1 Hz, $CH_{arom.}$), 8.10 (d, 1H, *J* = 6.9 Hz, $CH_{arom.}$), 8.04 (d, 1H, *J* = 8.2 Hz, $CH_{arom.}$), 7.83–7.75 (m, 2H, $CH_{arom.}$) ppm.

IV. Computational Methodology

All DFT calculation were carried out using B3LYP6-31G(d) in Gaussian 16.

Dihedral angle scans were calculated by geometry optimization with constrained central double bond of BANs.

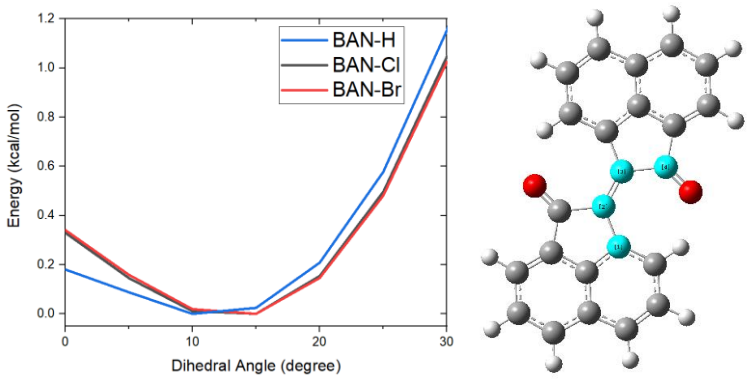


Figure S3. Dihedral angle scan of BANs with fixed dihedral angle (as labeled) from 0° to 30° by 5° increment.

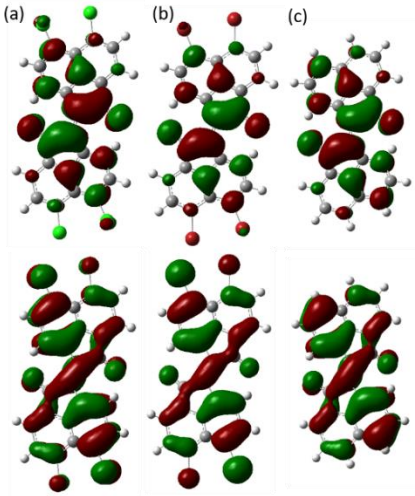


Figure S4. HOMO (down) and LUMO (up) orbital topology of fully optimized (a) BAN-Cl, (b) BAN-Br, (c) BAN-H.

Calculation of intramolecular reorganization energy (λ) for electron transport is decomposed into the geometric optimization, followed by vertical ionization of a neutral molecule, the geometric optimized of charged molecule, and then vertical neutralization of the charged molecule. The energy values are summarized in Table S1. Finally, λ is calculated by the following equations, where N is for neutral, '-' is for anionic molecule, v for vertical, and o for optimized state:

$$\lambda = \lambda_1 + \lambda_2$$

$$\lambda_1 = E_v(M^-) - E_o(M^-)$$

$$\lambda_2 = E_v(M_N) - E_o(M_N)$$

Table S1. Conformational energy of different states (eV).

	$E_o(M_N)$	$E_v(M^-)$	$E_o(M^-)$	$E_v(M_N)$	λ
BAN-H	-29177.297	-29178.600	-29178.830	-29177.070	0.457
BAN-Cl	-79201.612	-79203.517	-79203.752	-79201.383	0.464
BAN-Br	-309030.158	-309032.085	-309032.313	-309029.936	0.450

Electron coupling (charge integral, *t*) for electron transporting was calculated by the following equation, where E_L and E_{L+1} are the energies of the LUMO and LUMO+1 levels obtained from closed-shell configuration of a dimer based on its crystal structure:[8]

$$t = (E_{L+1}-E_L)/2$$

Table S2. Summary of energy states for charge integral calculation.

BAN-H	E_L (eV)	E_{L+1} (eV)	*t* (meV)
d_1	-2.564	-2.408	78
d_2	-2.758	-2.559	99
d_3	-2.799	-2.532	133
BAN-Cl	E_L (eV)	E_{L+1} (eV)	*t* (meV)
d_1	-3.153	-3.033	60
d_2	-3.113	-3.111	1
d_3	-3.134	-3.137	2
Cl…Cl	-3.087	-3.082	3
BAN-Br	E_L (eV)	E_{L+1} (eV)	*t* (meV)
d_1	-3.288	-3.173	58
d_2	-3.298	-3.283	8
d_3	-3.363	-3.189	87
Br···Br (3.60 Å)	-3.2665	-3.192	37
Br···Br (3.51 Å)	-3.251	-3.214	19

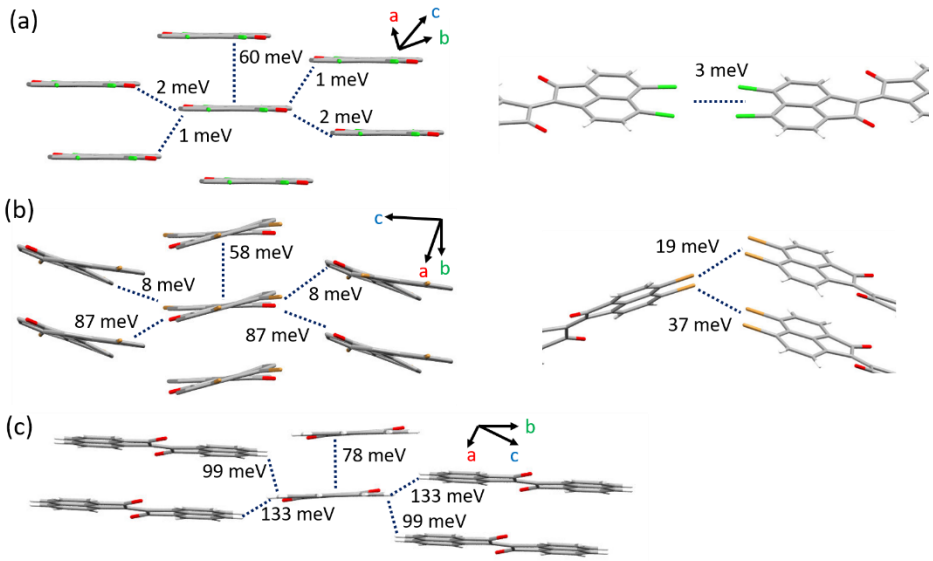


Figure S5. Calculated electron-transfer integral of (a) BAN-Cl, (b) BAN-Br, and (c) BAN-H, based on single-crystal structures.

V. Cyclic voltammetry

Due to poor solubility of BAN-Cl and BAN-Br, the compound was sublimed on Pt wire under vacuum of 10^{-5} mbar. BAN-Cl and BAN-Br had an irreversible reduction wave in acetonitrile. BAN-H was measured in CH_2Cl_2 solution, showing a reversible reduction wave.

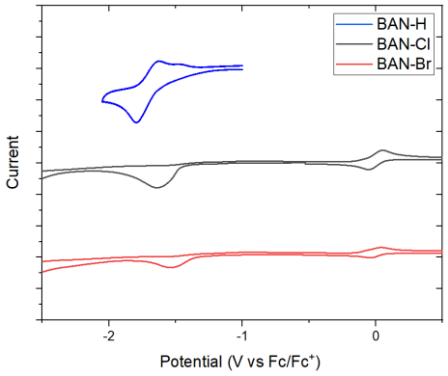


Figure S6. Cyclic voltammetry for BANs with ferrocene reference. E_{LUMO} of BAN-H was calculated by half-wave reduction potential vs. Fc/Fc^+, and E_{LUMO} of BAN-Cl and BAN-Br was by onset of reduction potential vs. Fc/Fc^+.

VI. Photoelectron Yield Spectroscopy in Air (PESA)

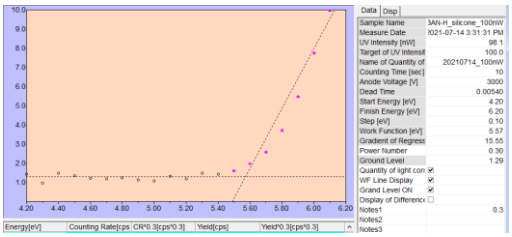


Figure S7. PESA of BAN-H film.

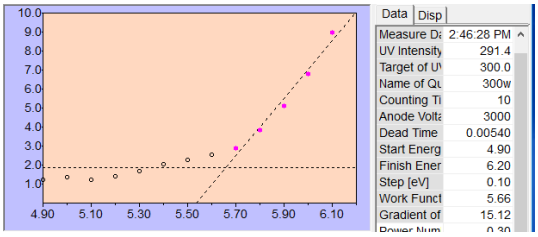


Figure S8. PESA of BAN-Cl thin film.

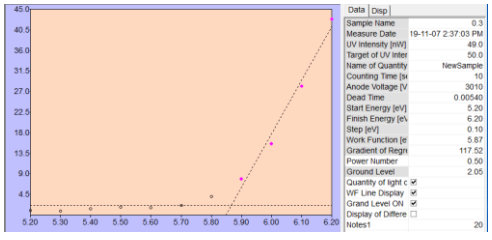


Figure S9. PESA of BAN-Br thin film.

VII. X-ray Crystallography

Single crystal X-ray diffraction (SCXRD): the data were measured on a Bruker D8 Venture diffractometer. The instrument is equipped with a Photon 200 area detector, and IμS microfocus X-ray source (Bruker AXS, Cu*K*α source, λ = 1.54184 Å). All measurements were carried out at room temperature for BAN-Cl and BAN-Br, but for BAN-H was collected at 173(2)K. Crystals were coated with a thin layer of amorphous Paratone oil in order to decrease crystal deterioration, structural disorder, or any related thermal motion effects and to improve the accuracy of the structural results. Structure solution was carried out using the SHELXTL package from Bruker.[9] The parameters were refined for all data by full-matrix-least-squares or F^2 using SHELXL.[10] All of the nonhydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atom thermal parameters were constrained to ride on the carrier atom.

Table S3. X-ray diffraction data of BAN-Cl, BAN-Br, and BAN-H.

Compound	BAN-H	BAN-Cl	BAN-Br
Identification code	2101214	2087155	2087157
Empirical formula	$C_{24}H_{12}O_2$	$C_{24}H_8Cl_4O_2$	$C_{24}H_8Br_4O_2$
Formula weight	332.34	470.10	647.94
Temperature/K	173(2)	298(2)	298(2)
Crystal system	monoclinic	triclinic	orthorhombic
Space group	$P2_1/c$	P-1	$Pna2_1$
a/Å	3.8029(3)	3.8349(4)	31.7745(16)
b/Å	13.8237(10)	8.8365(7)	3.8742(2)
c/Å	14.1694(10)	13.2606(9)	15.4074(10)
α/°	90	88.717(5)	90
β/°	94.395(5)	89.773(6)	90
γ/°	90	78.865(6)	90
Volume/Å^3	742.70(10)	440.79(7)	1896.66(18)
Z	2	1	4
ρ_{calc}g/cm^3	1.486	1.771	2.269
μ/mm^{-1}	0.747	6.291	10.539
F(000)	344.0	236.0	1232.0
2θ range for data collection/°	8.95 to 144.976	6.668 to 144.894	5.562 to 144.9
Index ranges	$-4 \le h \le 4$, $-17 \le k \le 17$, $-17 \le l \le 17$	$-4 \le h \le 4$, $-10 \le k \le 10$, $-16 \le l \le 16$	$-39 \le h \le 39$, $-3 \le k \le 4$, $-19 \le l \le 19$
Reflections collected	10769	12693	25266
Independent reflections	1475 [R_{int} = 0.0928, R_{sigma} = 0.0501]	1722 [R_{int} = 0.0443, R_{sigma} = 0.0255]	3746 [R_{int} = 0.1123, R_{sigma} = 0.0605]
Data/restraints/parameters	1475/0/118	1722/0/136	3746/1/272
Goodness-of-fit on F^2	1.045	1.021	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0519, wR_2 = 0.1190	R_1 = 0.0331, wR_2 = 0.0975	R_1 = 0.0582, wR_2 = 0.1448
Final R indexes [all data]	R_1 = 0.0750, wR_2 = 0.1407	R_1 = 0.0350, wR_2 = 0.1011	R_1 = 0.0805, wR_2 = 0.1648
Largest diff. peak/hole / e Å^{-3}	0.21/-0.19	0.31/-0.31	0.71/-1.00

VIII. NMR Spectra

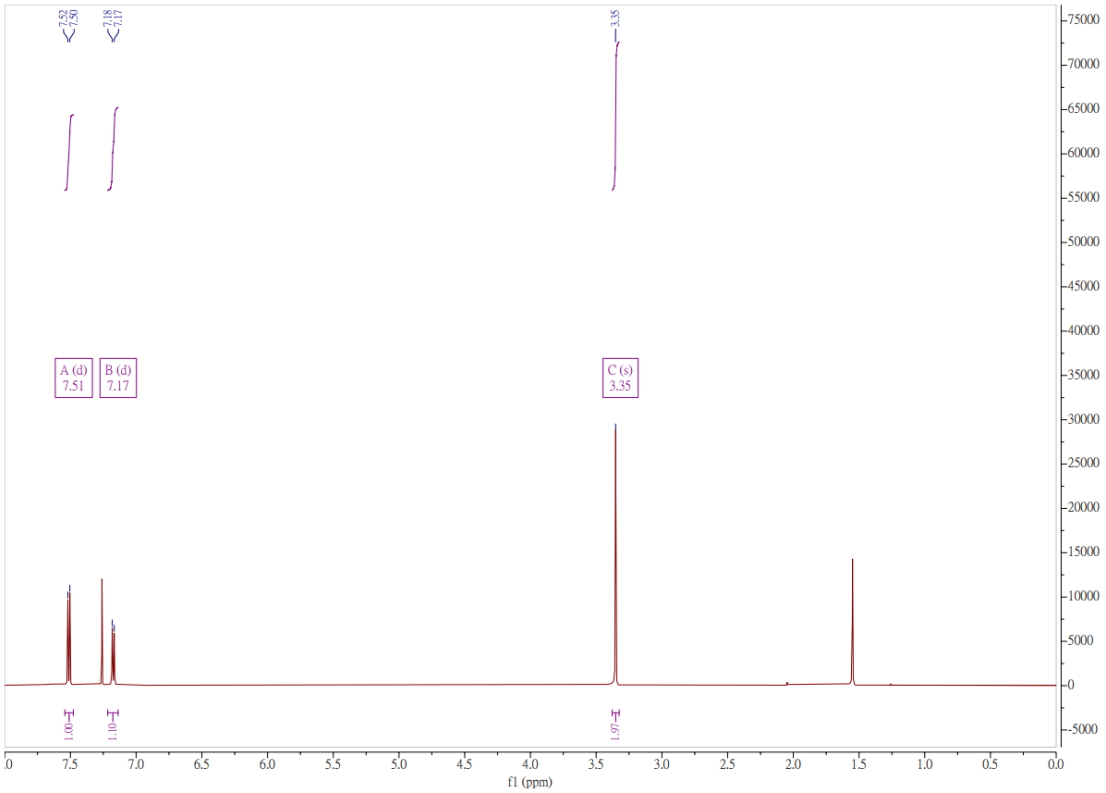


Figure S10. ^{1}H-NMR of 5,6-dichloro-1,2-dihydroacenaphthylene (**1**) ($CDCl_3$, 25 °C).

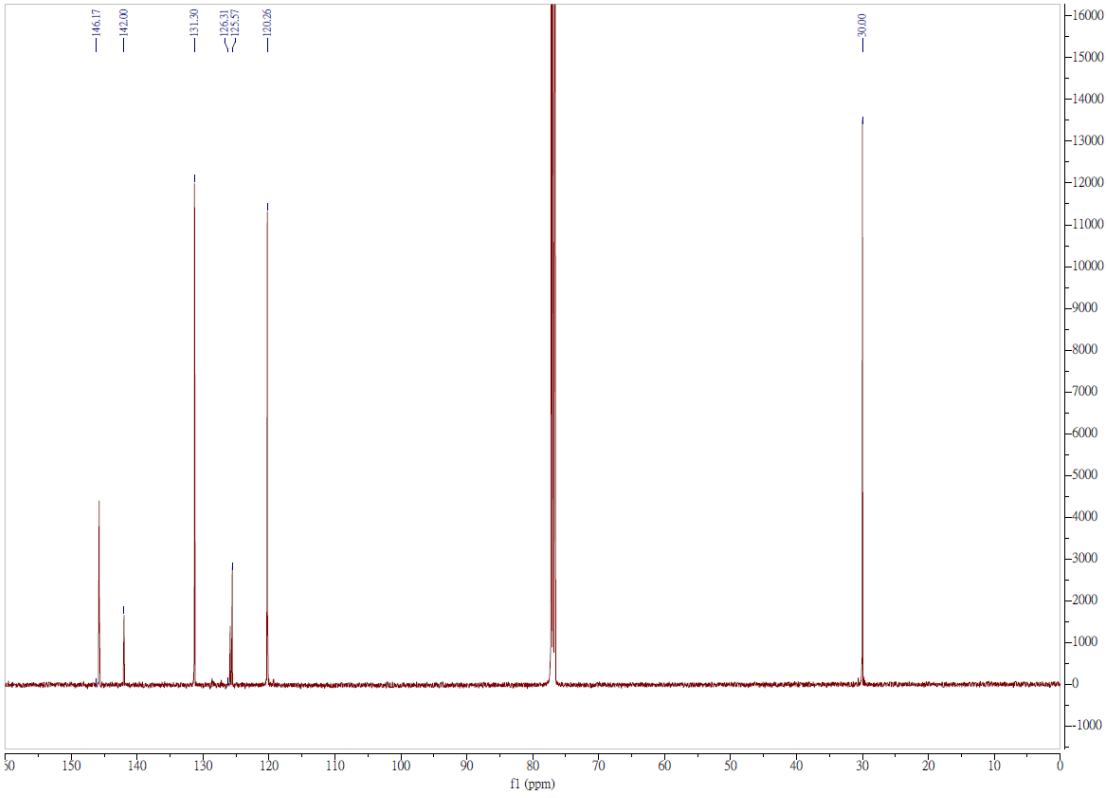


Figure S11. ^{13}C-NMR of 5,6-dichloro-1,2-dihydroacenaphthylene (**1**) ($CDCl_3$, 25 °C).

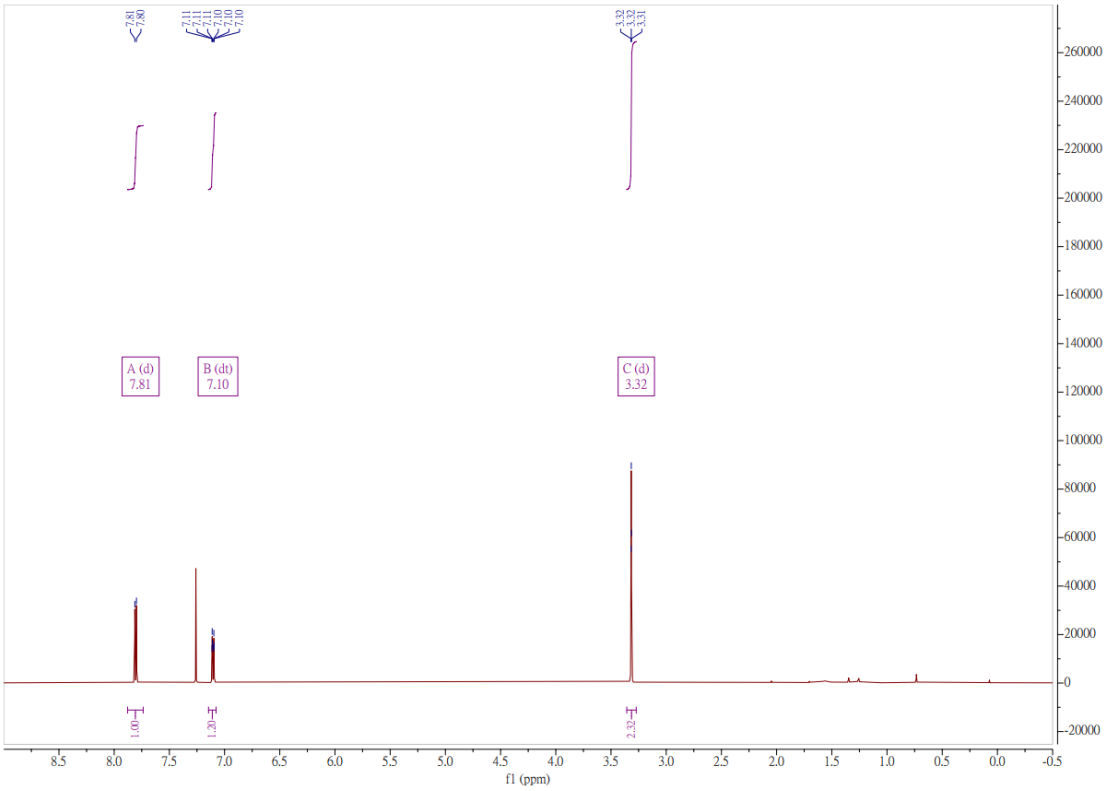


Figure S12. ^{1}H-NMR of 5,6-dibromo-1,2-dihydroacenaphthylene (**2**) ($CDCl_3$, 25 °C).

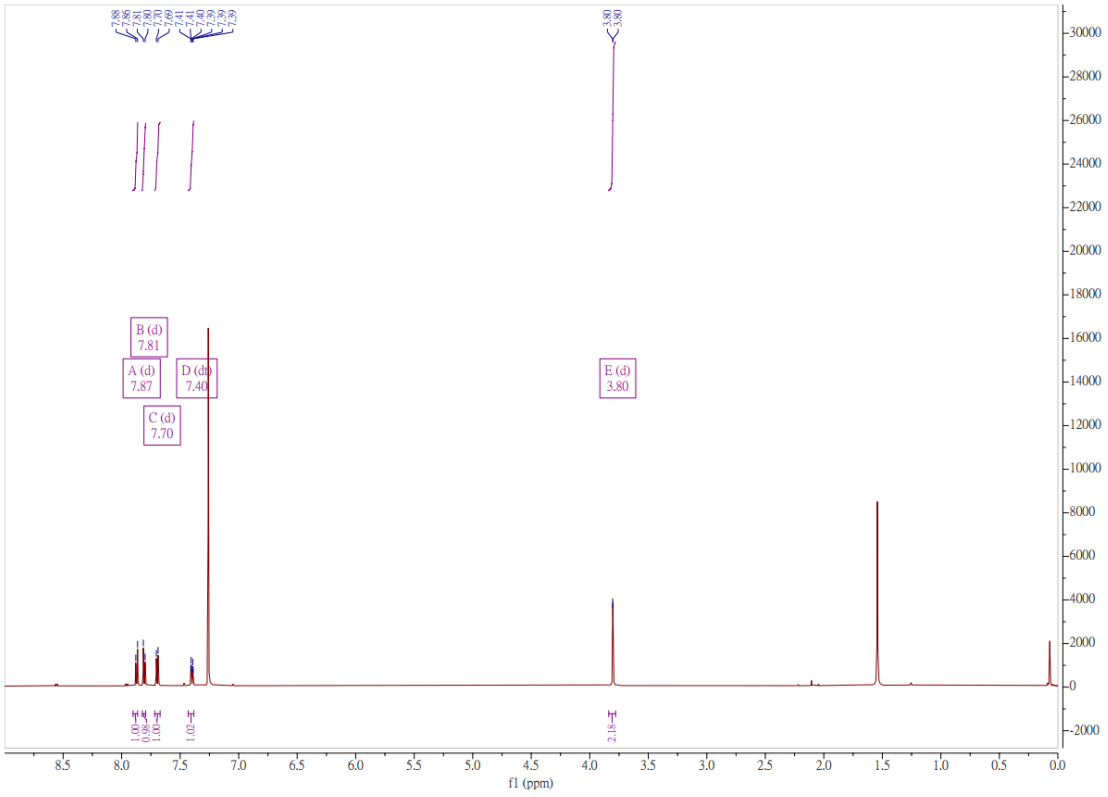


Figure S13. ^{1}H-NMR of 5,6-dichloroacenaphthylen-1(2*H*)-one (**3**) ($CDCl_3$, 25 °C).

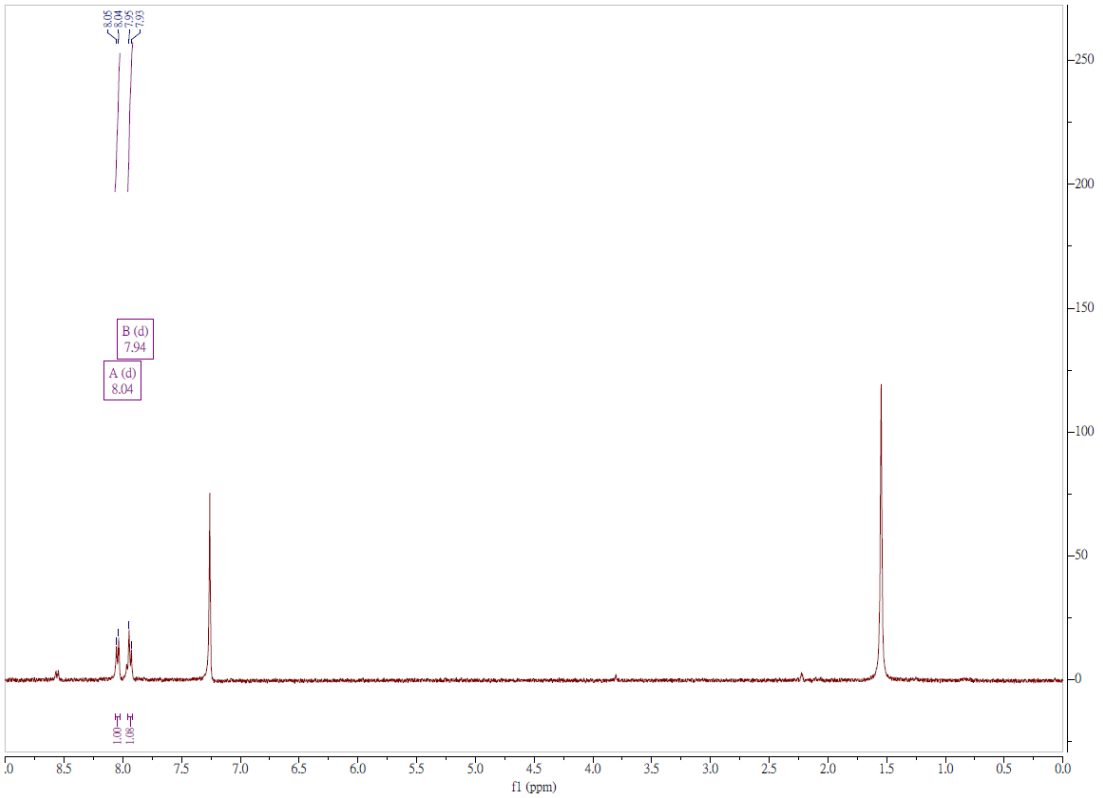


Figure S14. ^{1}H-NMR of 5,6-dichloroacenaphthylene-1,2-dione (**4**) ($CDCl_3$, 25 °C).

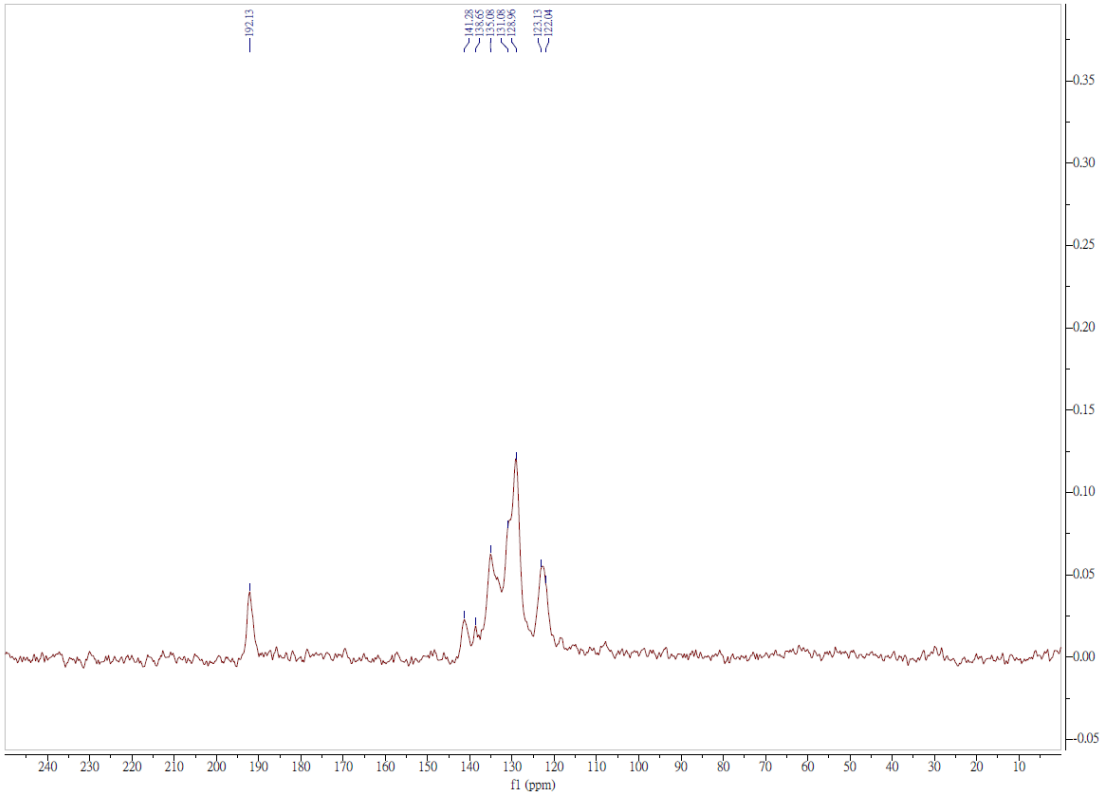


Figure S15. Solid-state NMR of BAN-Cl.

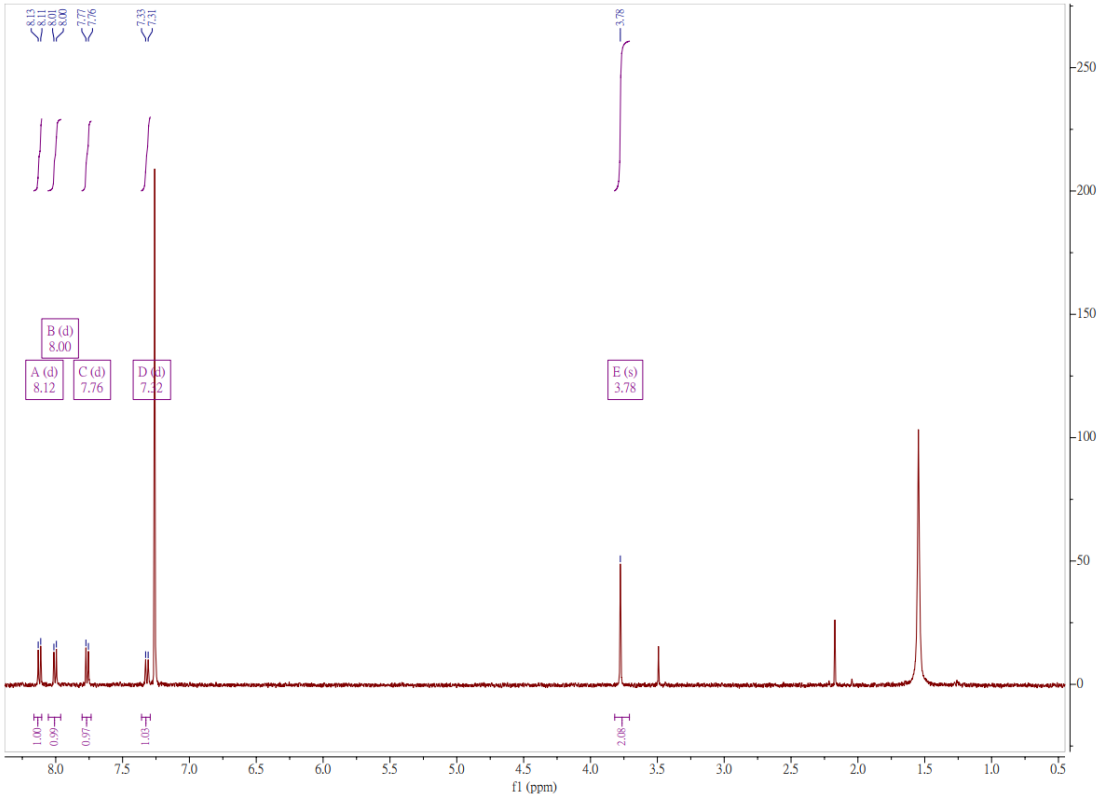


Figure S16. ^{1}H-NMR of 5,6-dibromoacenaphthylen-1(2*H*)-one (**5**) ($CDCl_3$, 25 °C).

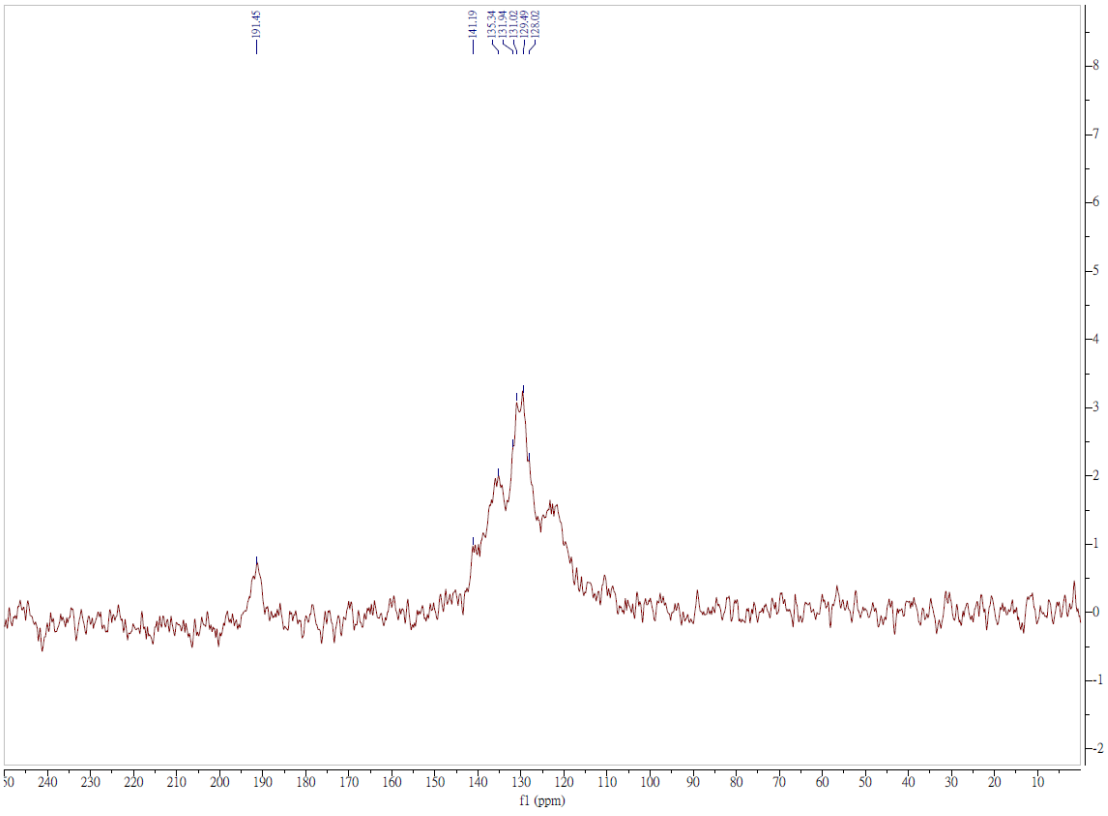


Figure S17. Solid-state NMR of BAN-Br.

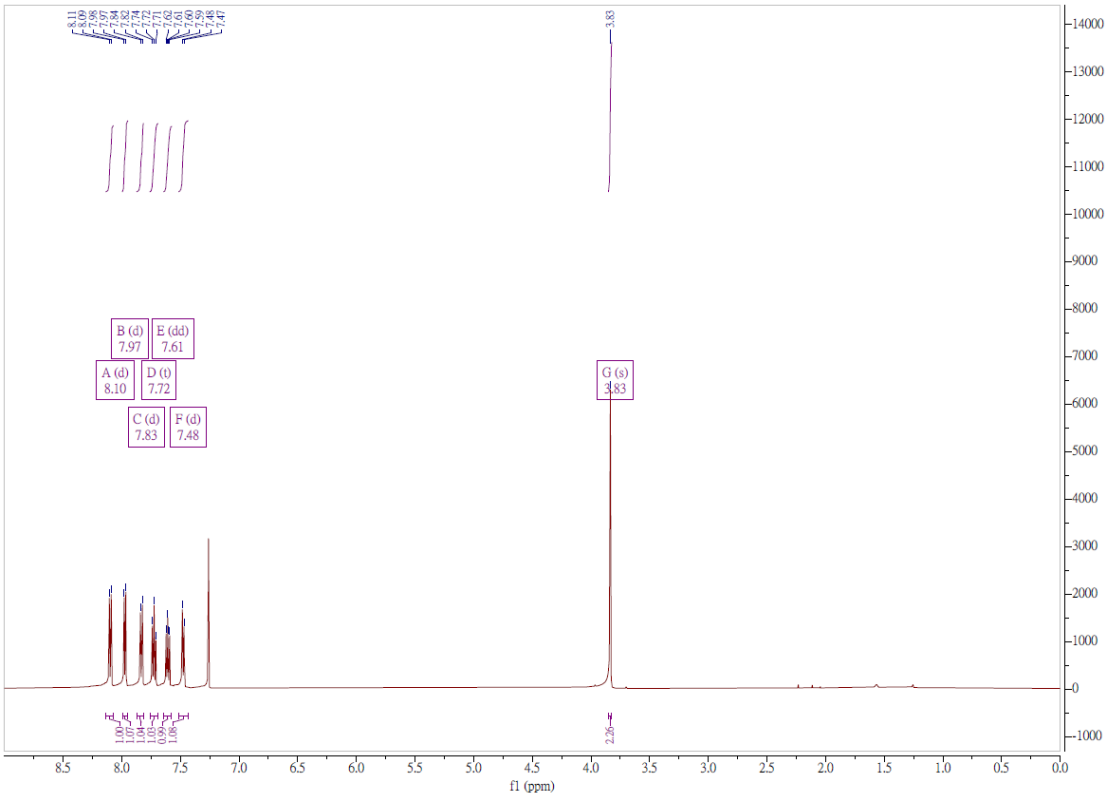


Figure S18. ^{1}H-NMR of acenaphthylen-1(2*H*)-one (**7**) ($CDCl_3$, 25 °C).

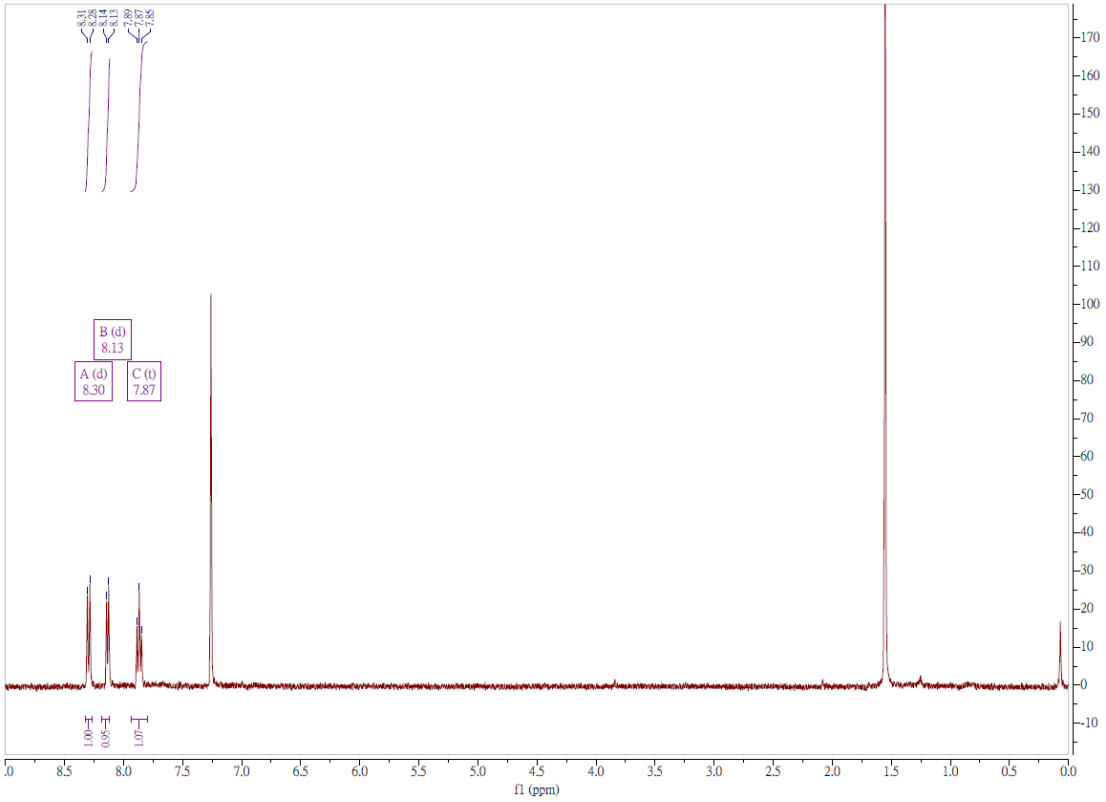


Figure S19. ^{1}H-NMR of acenaphthylene-1,2-dione (**8**) ($CDCl_3$, 25 °C).

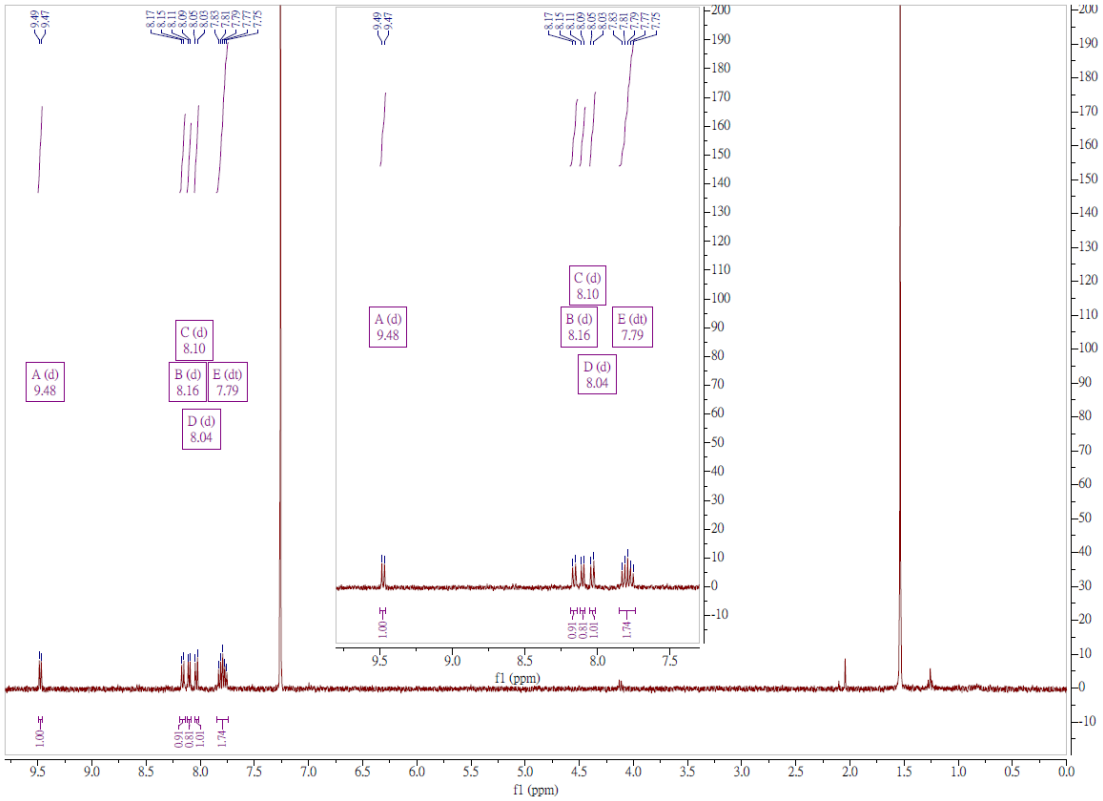


Figure S20. ^{1}H-NMR of BAN-H ($CDCl_3$, 25 °C).

IX. Infrared Spectra of BAN derivatives

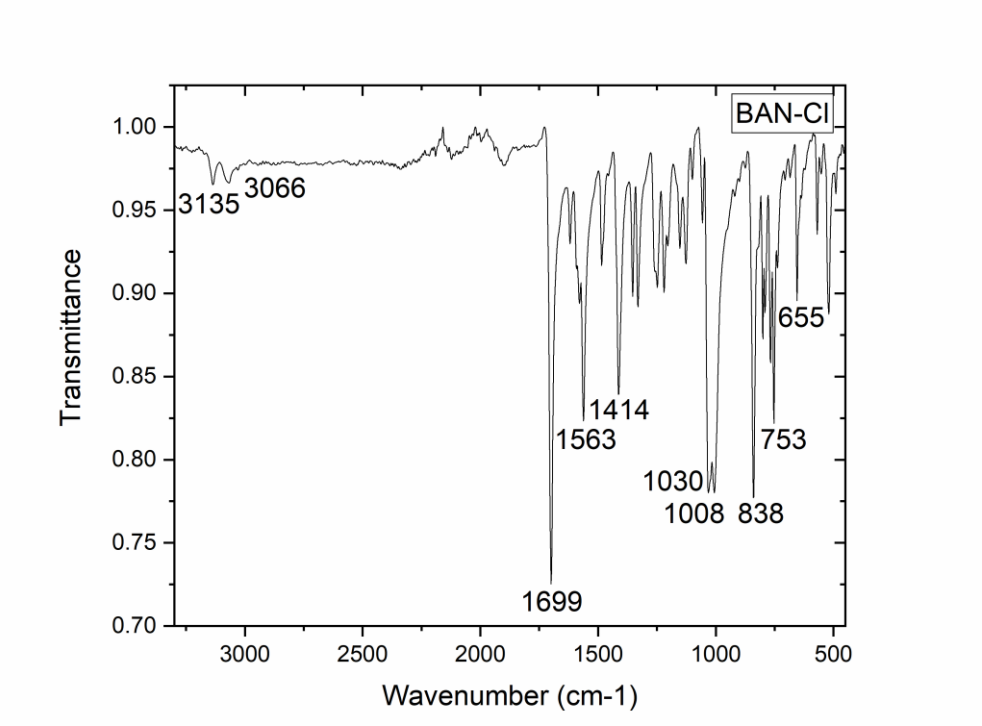


Figure S21. FTIR of BAN-Cl powder.

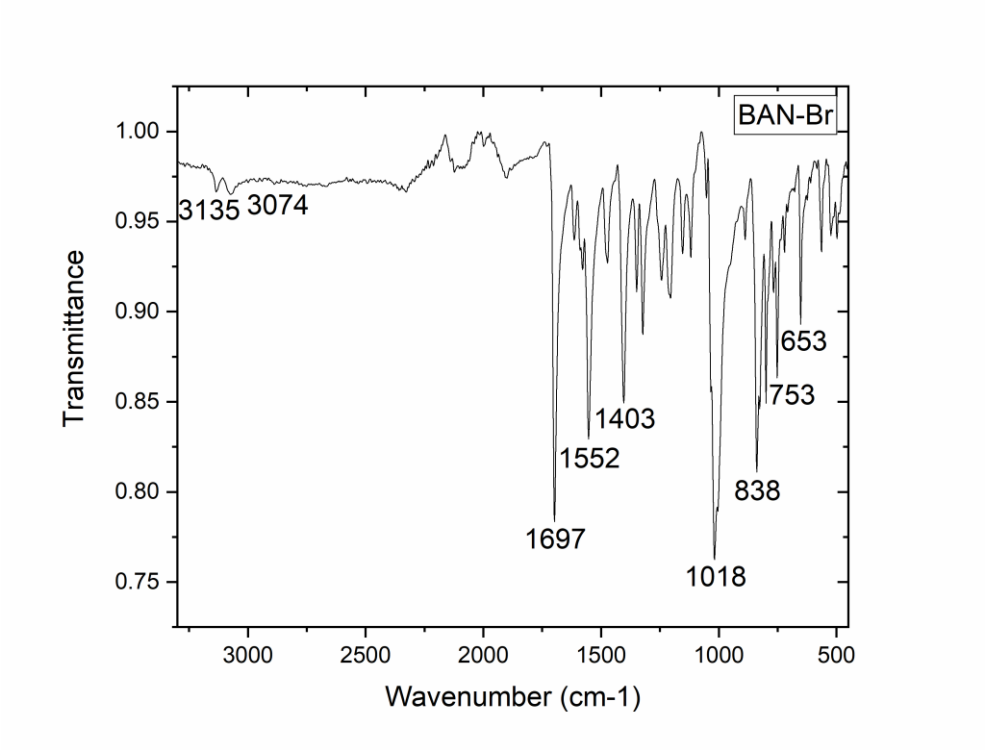


Figure S22. FTIR of BAN-Br powder.

X. Thermogravimetric Analysis

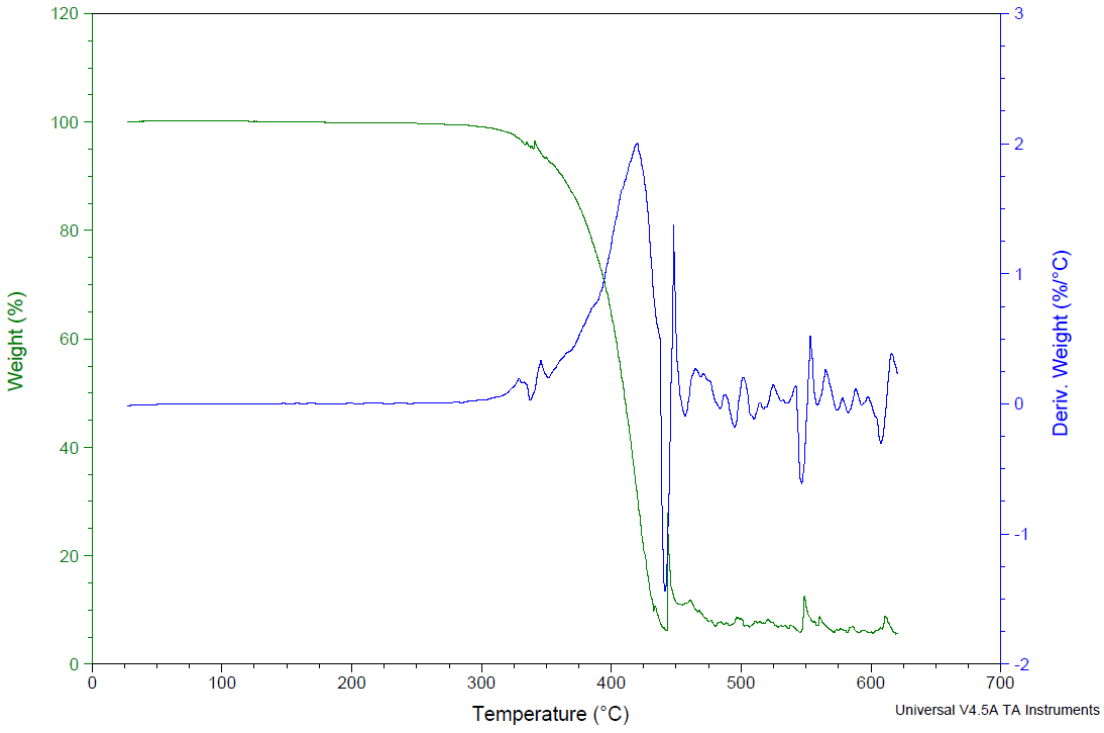


Figure S23. TGA of BAN-Cl under nitrogen atmosphere.

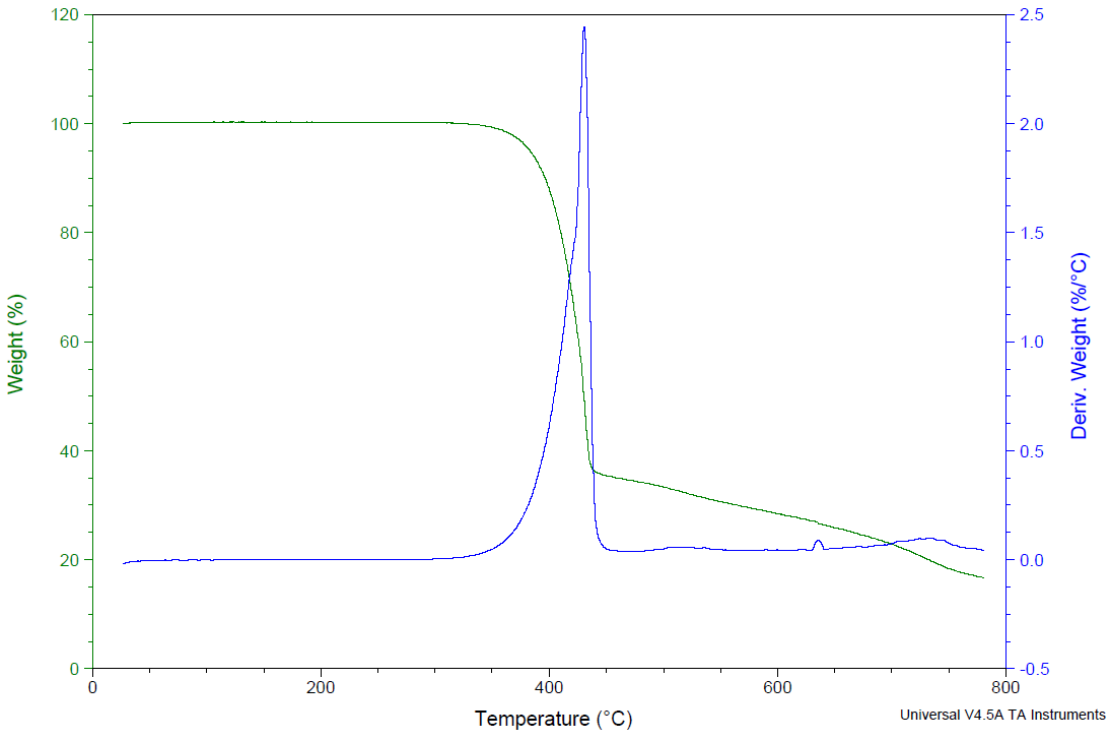


Figure S24. TGA of BAN-Br under nitrogen atmosphere.

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