Supporting Information

for

Molecular engineering of π-extended pyrrolo[1,2-*α*]quinoxaline-based D-A materials for electrochromic devices

Kexin Zhao [a,b], Wenquan Wang [a,b], Chengyi Kang [a,b], Ziyi Zhang [a,b], Haitao Xu [a,b], Quan Liu [*a,b], Huiping Dai[*c]

[a] Shaanxi Province Key Laboratory of Catalytic, Shaanxi University of Technology, Hanzhong 723001, P. R. China.

[b] School of Chemical and Environmental Science, Shaanxi University of Technology, Hanzhong 723001, P. R. China.

[c] School of Biolegical Science and Engineering, Shaanxi University of Technology, Hanzhong 723001, P. R. China.

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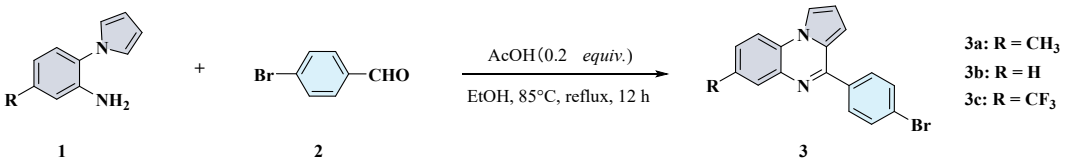
1. Synthesis and characterization

1.1 Synthesis of compounds 3a, 3b and 3c



1 2 3

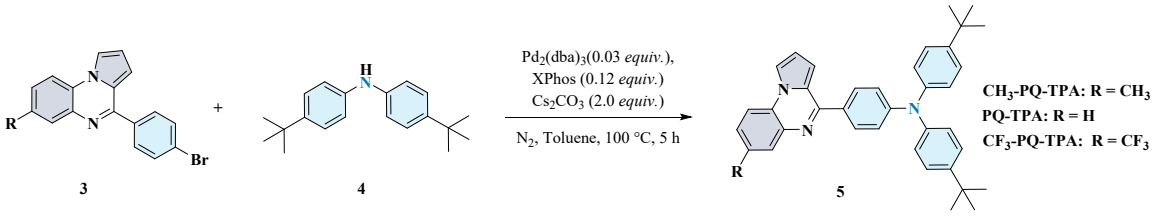
A mixture of various substituted **1** (3.0 mmol), 4-bromobenzaldehyde **2** (3.0 mmol, 1.0 *equiv.*), EtOH (10 mL) were added to a round-bottomed flask (25 mL). After AcOH (0.6 mmol, 36 mg, 0.2 *equiv.*) was added. Then the reaction mixture was heated up to 85 °C and stirred for 12 h. After completion of the reaction, the solvent evaporation under reduced pressure, the residue was purified by column chromatography on silica gel to afford the product **3**.

3a: white solid (726 mg, yield 75%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ*: 7.95 (dd, *J* = 2.9, 1.3 Hz, 1H), 7.91 ~ 7.85 (m, 2H), 7.84 ~ 7.80 (m, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.70 ~ 7.64 (m, 2H), 7.33 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.92 (dd, *J* = 4.1, 1.3 Hz, 1H), 6.87 (dd, *J* = 4.1, 2.7 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) *δ*: 153.0, 137.4, 136.1, 135.2, 131.7, 130.2, 130.0, 128.8, 125.0, 124.9, 124.0, 114.5, 113.8, 113.4, 108.1, 21.1. HRMS-ESI (m/z) calcd. for $C_{18}H_{13}BrN_2$ $[M+H]^+$: 337.0262; found: 337.0257.

3b: white solid (657 mg, yield 65%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ*: 8.05 ~ 7.99 (m, 2H), 7.88 (t, *J* = 6.9 Hz, 3H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.3 Hz, 1H), 6.96 (d, *J* = 3.5 Hz, 1H), 6.92 ~ 6.89 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) *δ*: 153.2, 137.3, 136.1, 131.8, 130.3, 127.8, 127.2, 125.5, 125.0, 124.2, 114.9, 114.2, 113.7, 108.6. HRMS-ESI (m/z) calcd. for $C_{17}H_{11}BrN_2$ $[M+H]^+$: 323.0106; found: 323.0180

3c: white solid (739 mg, yield 64%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ*: 8.31 (s, 1H), 8.04 (s, 1H), 7.96 (dd, *J* = 8.6, 3.1 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.6 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 4.0 Hz, 1H), 6.97 (d, *J* = 3.9 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) *δ*: 154.5, 136.8, 135.9, 131.9, 130.2, 129.2, 127.8, 127.8, 127.5, 125.1, 124.8, 124.7, 124.0, 124.0, 124.0, 123.0, 115.6, 115.1, 114.4, 109.6. HRMS-ESI (m/z) calcd. for $C_{18}H_{10}BrF_3N_2$ $[M+H]^+$: 390.9979; found: 391.0040.

1.2 Synthesis of compounds CH_3-PQ-TPA, PQ-TPA and CF_3-PQ-TPA



3 4 5

Under nitrogen protection, a mixture of **3** (0.5 mmol), 4,4'-di-*tert*-butyldiphenylamine **4** (0.5 mmol, 1.1 *equiv.*), Cs_2CO_3 (325.8 mg, 1.0 mmol, 2.0 *equiv.*), $Pd_2(dba)_3$ (14 mg, 0.015 mmol, 0.03 *equiv.*), XPhos (28.6 mg, 0.06 mmol, 0.12 *equiv.*) and toluene (10 mL) were added to a sealing tube. Then, the reaction mixture was heated up to 100 °C and stirred for 5 h. Next, the reaction was quenched with brine, extracted by dichloromethane and dried by anhydrous Na_2SO_4. After the solvent evaporation under reduced pressure, the residue was purified by column chromatography on silica gel (PE: DCM= 1:1) to afford the product.

CH_3-PQ-TPA: yellow solid (228 mg, 85%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ*: 7.94 (dd, *J* = 2.8, 1.3 Hz, 1H), 7.90 ~ 7.86 (m, 2H), 7.83 (t, *J* = 1.5 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 2.3 Hz, 2H), 7.30 (q, *J* = 2.8, 2.3 Hz, 3H), 7.19 ~ 7.16 (m, 2H), 7.14 ~ 7.09 (m, 4H), 7.04 (dd, *J* = 4.1, 1.3 Hz, 1H), 6.86 (dd, *J* = 4.0, 2.7 Hz, 1H), 2.50 (s, 3H), 1.34 (s, 18H). ^{13}C NMR (101 MHz, Chloroform-*d*) *δ*: 153.8, 149.7, 146.3, 144.7, 136.3, 134.9, 131.2, 129.8, 129.4, 128.1, 126.1, 125.3, 124.9, 124.6, 121.7, 114.2, 113.5, 113.3, 108.3, 34.3, 31.4, 21.1. HRMS-ESI (m/z) calcd. for $C_{38}H_{39}N_3$ $[M+H]^+$: 538.3144; found: 538.3146.

PQ-TPA: yellow solid (209 mg, 80%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ:* 8.03 (d, *J* = 7.7 Hz, 1H), 8.00 ~ 7.97 (m, 1H), 7.88 (t, *J* = 9.1 Hz, 3H), 7.52 ~ 7.41 (m, 2H), 7.31 (d, *J* = 8.6 Hz, 4H), 7.18 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 4H), 7.07 (d, *J* = 3.7 Hz, 1H), 6.91 ~ 6.87 (m, 1H), 1.34 (s, 18H). ^{13}C NMR (100 MHz, Chloroform-*d*) *δ:*154.0, 149.9, 146.4, 144.6, 130.0, 129.5, 129.0, 127.1, 126.2, 125.4, 125.3, 124.6, 121.7, 114.5, 113.9, 113.6, 108.7, 34.4, 31.5. HRMS-ESI (m/z) calcd. for $C_{37}H_{37}N_3$ $[M+H]$+: 524.2987; found: 524.3058.

CF_3-PQ-TPA: yellow solid (266 mg, 90%), ^{1}H NMR (400 MHz, Chloroform-*d*) *δ*: 8.29 (s, 1H), 8.00 (s, 1H), 7.93 (d, *J* = 8.6 Hz, 1H), 7.90 ~ 7.87 (m, 2H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.0 Hz, 5H), 7.16 (dd, *J* = 8.7, 1.9 Hz, 3H), 7.11 (dd, *J* = 8.6, 1.9 Hz, 6H), 6.94 (dt, *J* = 4.1, 2.3 Hz, 1H), 1.34 (d, *J* = 2.0 Hz, 18H). ^{13}C NMR (100 MHz, Chloroform-*d*) *δ*: 155.2, 150.3, 146.7, 144.5, 136.2, 130.2, 129.5, 129.1, 127.5(d, *J* = 4.4 Hz), 127.5, 126.2, 125.5, 124.8, 123.2(d, *J* = 3.8 Hz), 123.2, 121.3, 117.4, 115.1, 114.7, 114.2, 109.7, 34.4, 31.4. HRMS-ESI (m/z) calcd. for $C_{38}H_{36}F_3N_3$ $[M+H]^+$: 592.2861; found: 592.2940.

1.3 NMR Spectra

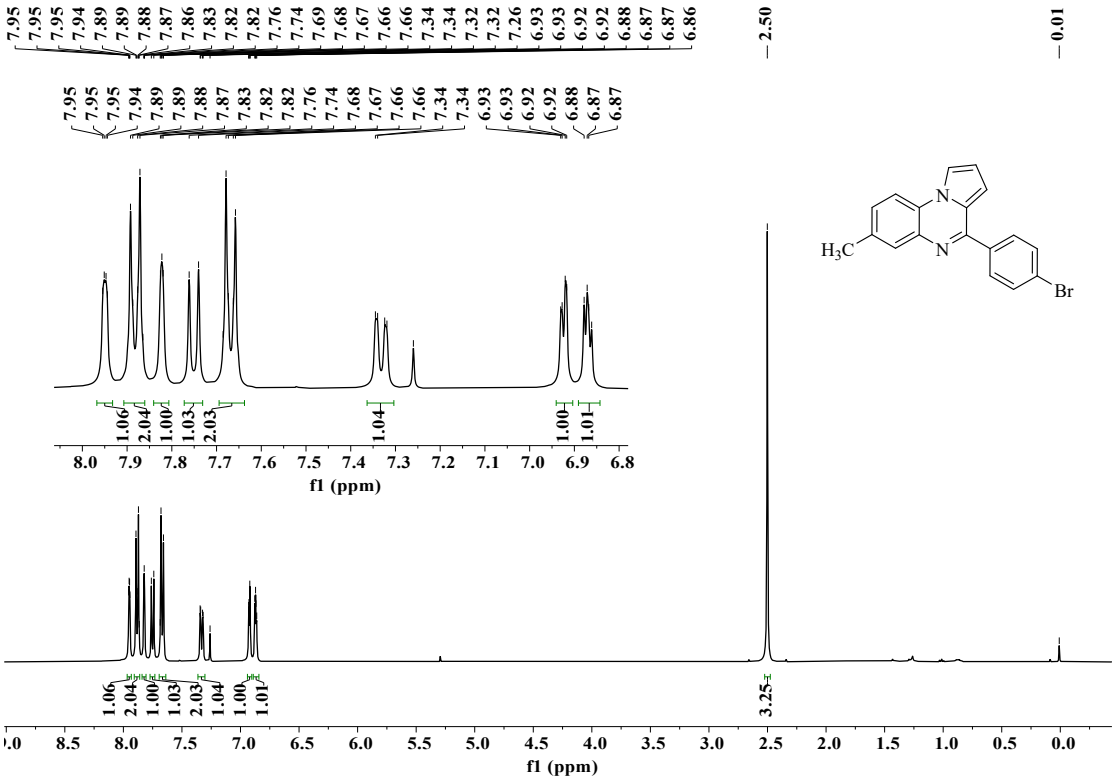


Fig. S1 ^{1}H NMR (400 MHz, Chloroform-*d*)

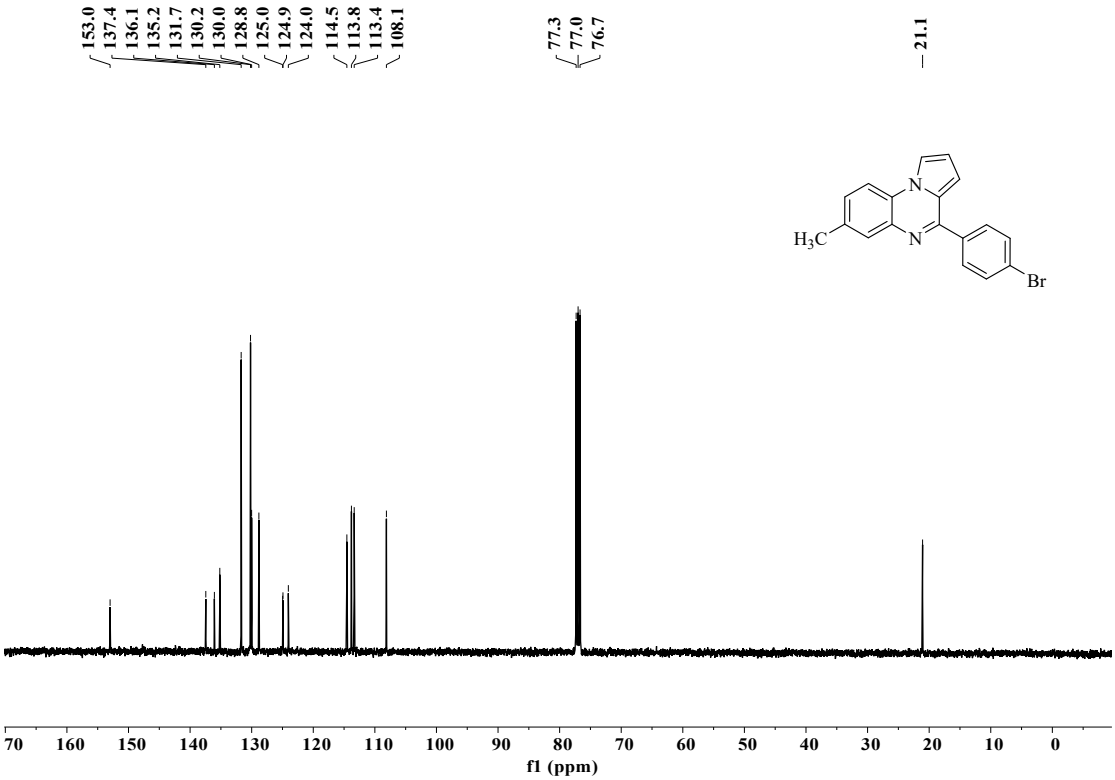


Fig. S2 ^{13}C NMR (100 MHz, Chloroform-*d*)

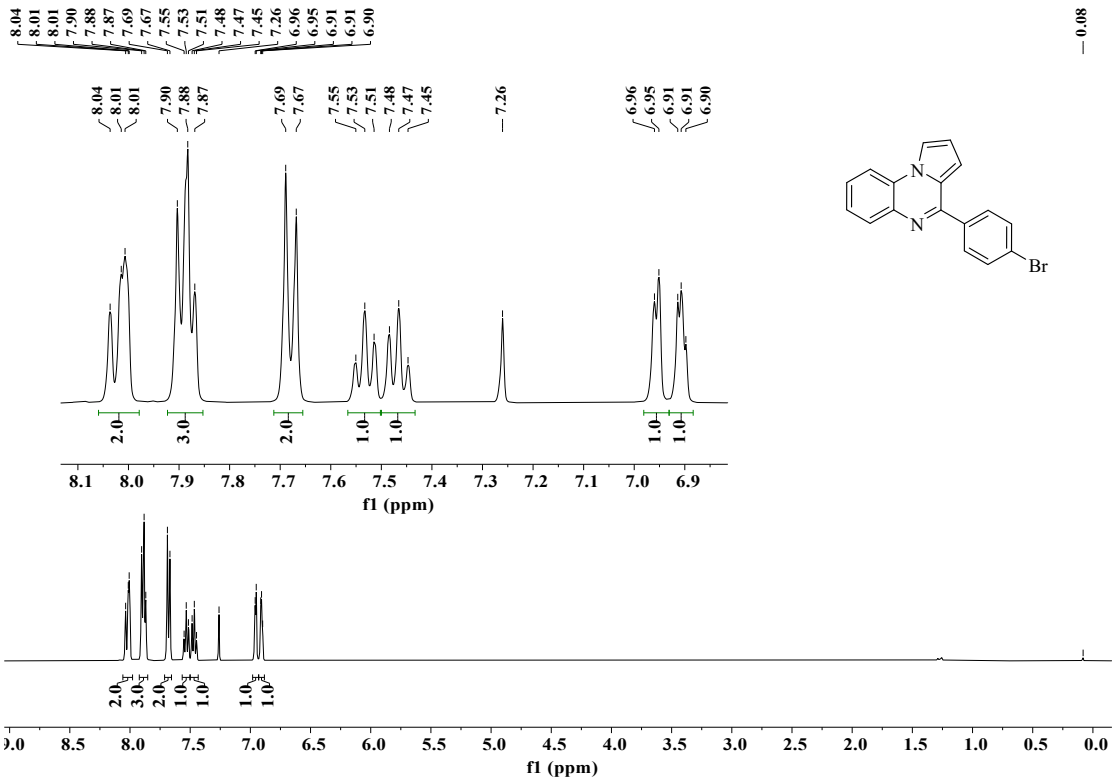


Fig. S3 ^{1}H NMR (400 MHz, Chloroform-*d*)

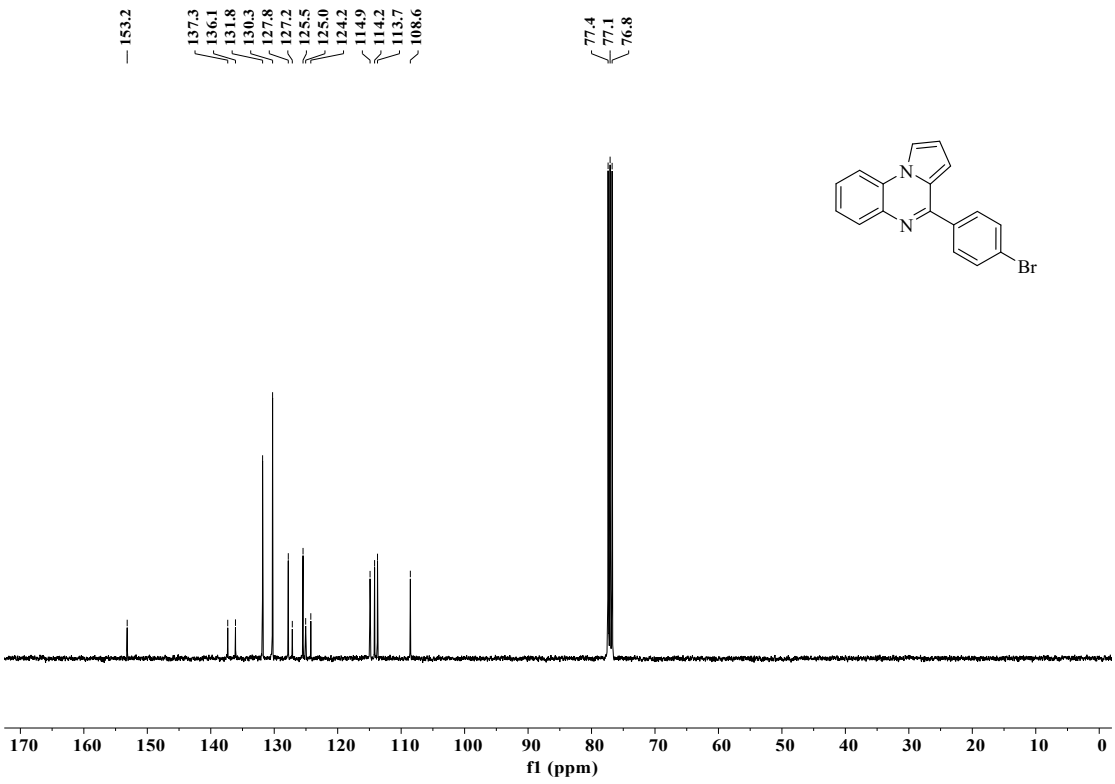


Fig. S4 ^{13}C NMR (100 MHz, *Chloroform-d*)

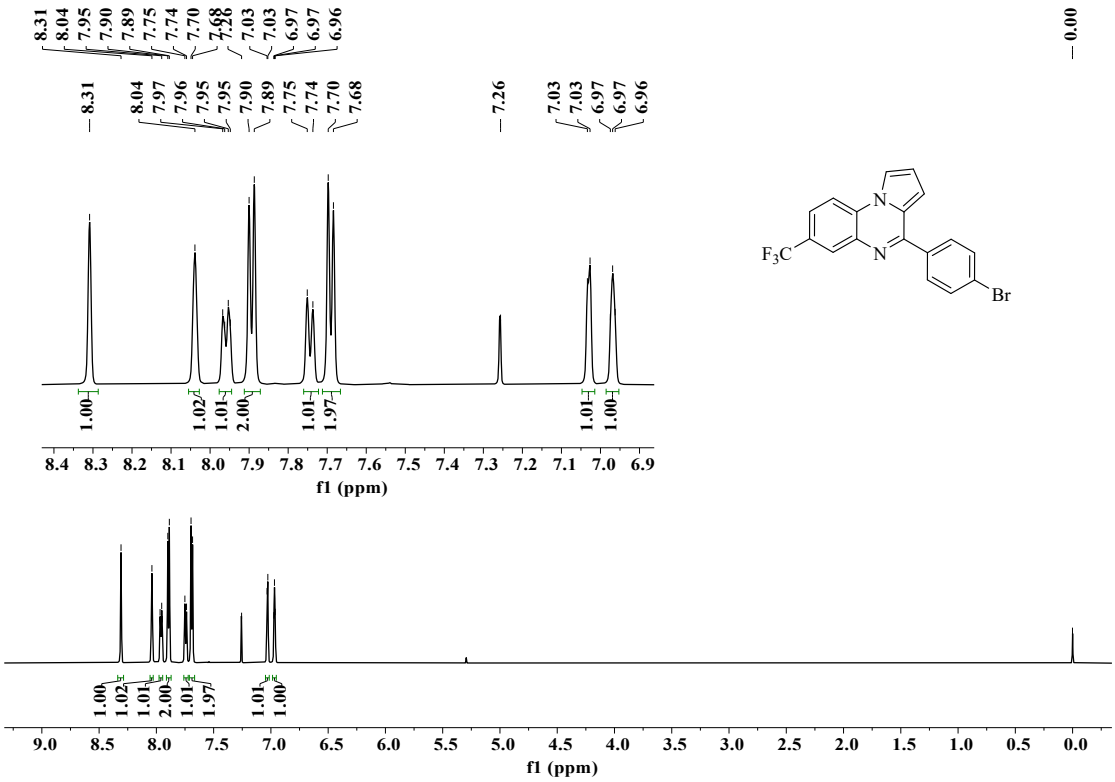


Fig. S5 ^{1}H NMR (400 MHz, *Chloroform-d*)

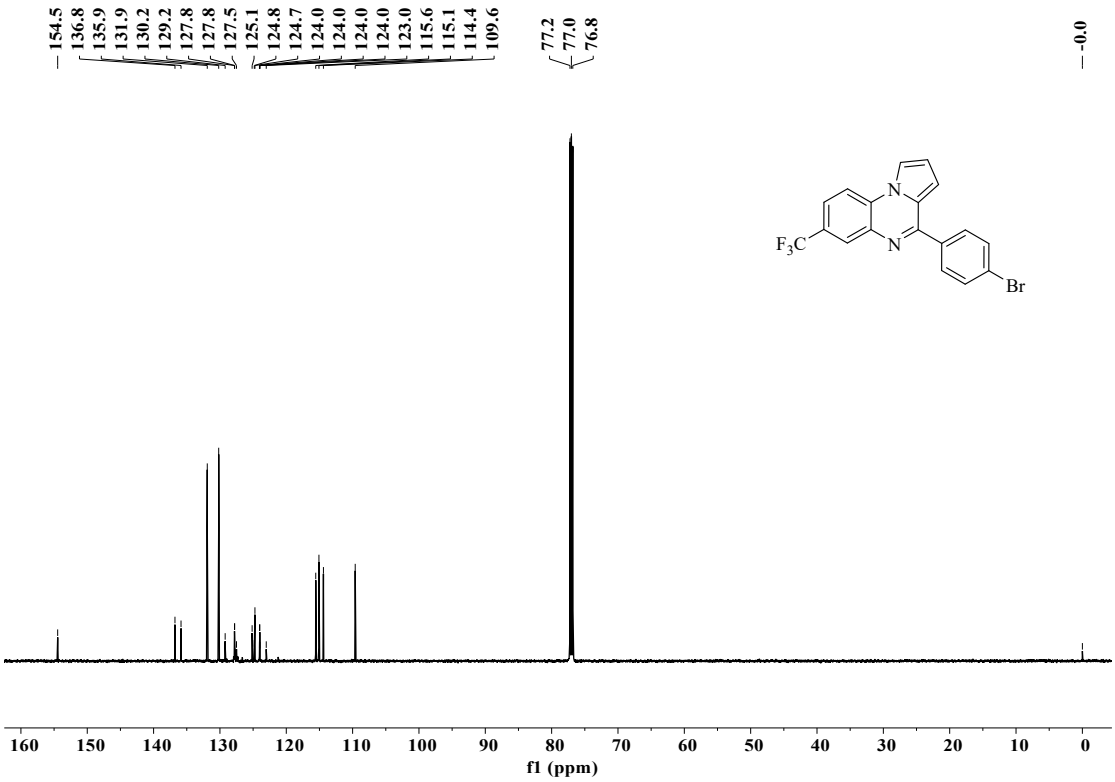


Fig. S6 ^{13}C NMR (100 MHz, *Chloroform-d*)

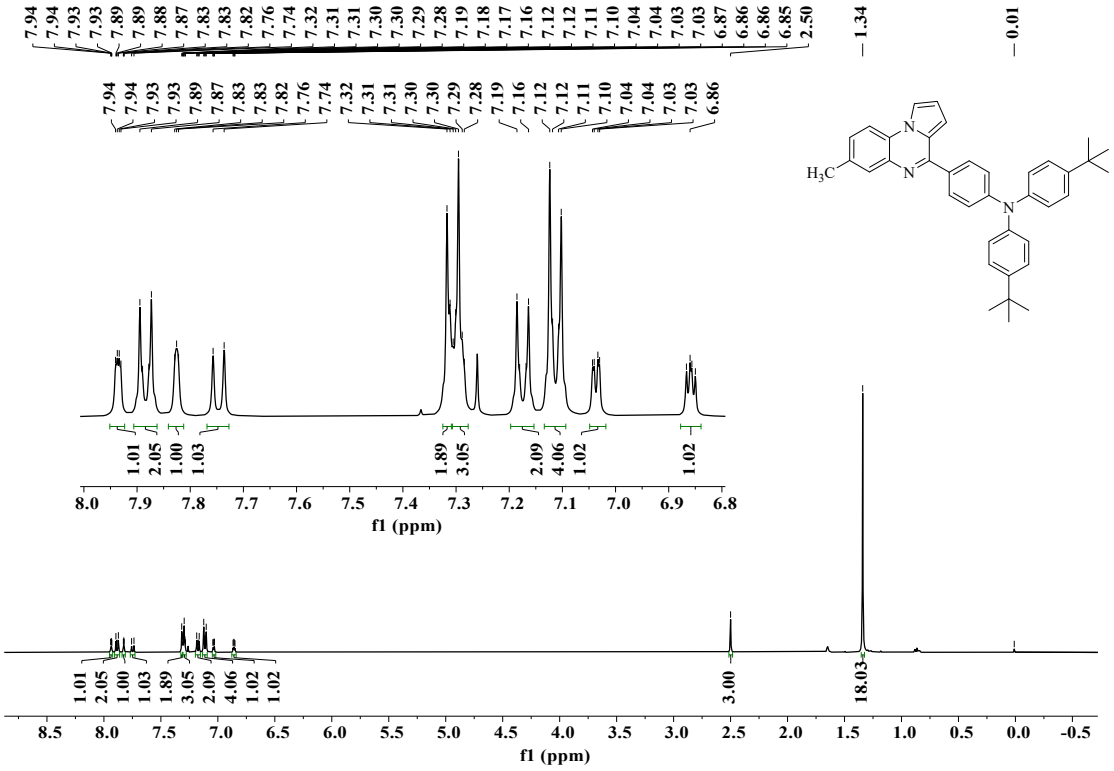


Fig. S7 ^{1}H NMR (400 MHz, *Chloroform-d*)

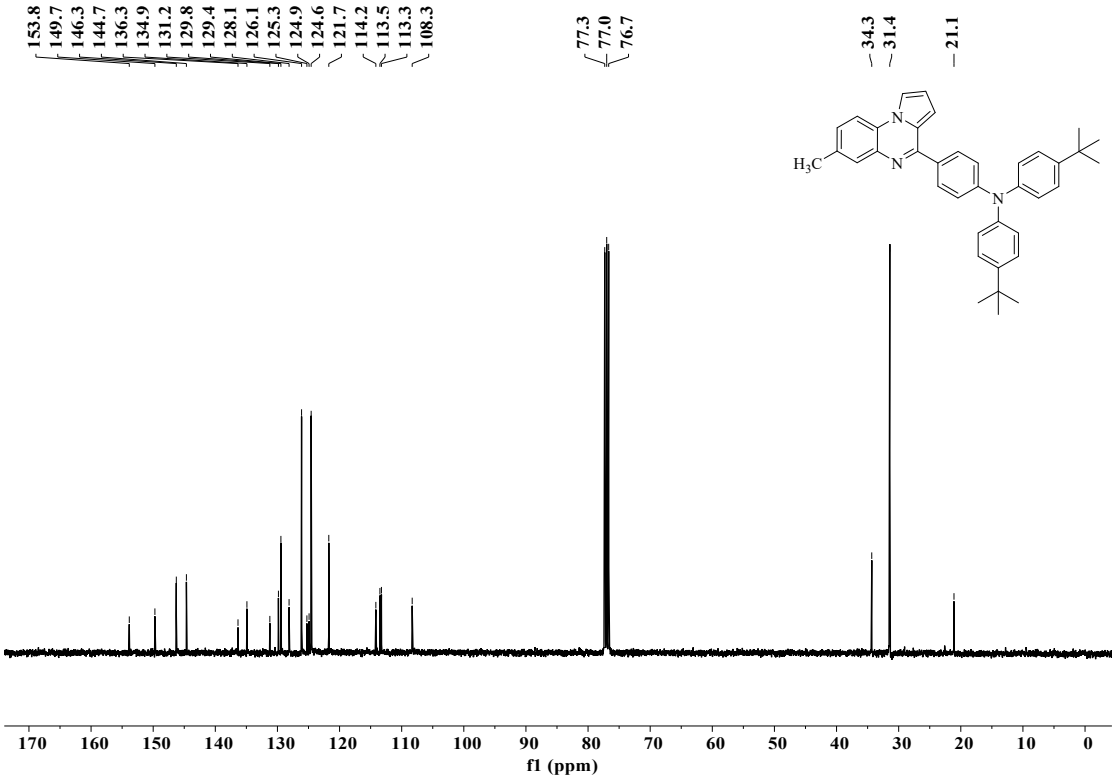


Fig. S8 ^{13}C NMR (100 MHz, Chloroform-d)

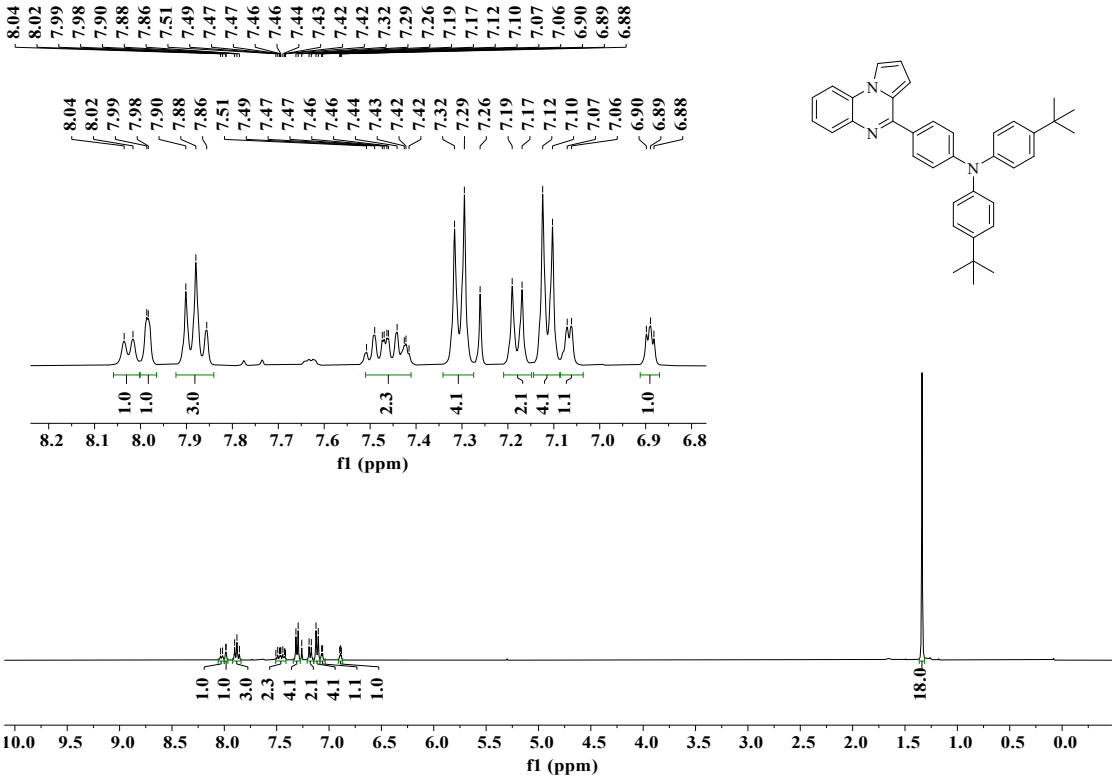


Fig. S9 ^{1}H NMR (400 MHz, *Chloroform-d*)

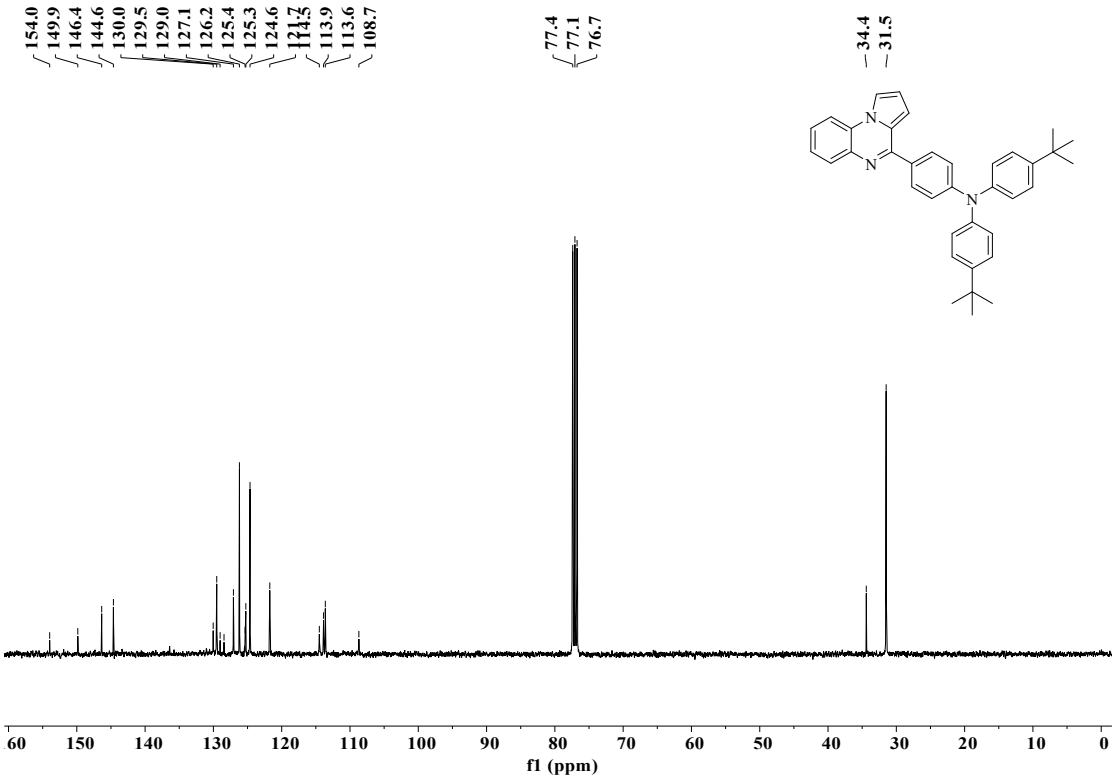


Fig. S10 ^{13}C NMR (100 MHz, Chloroform-*d*)

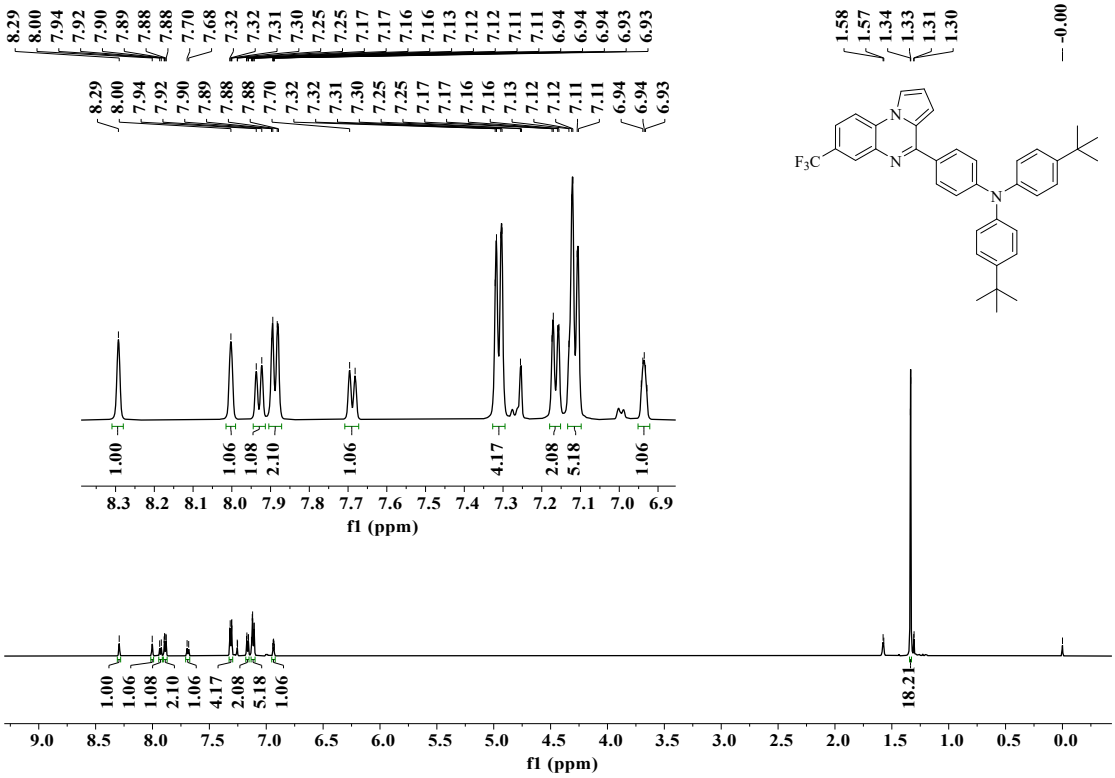


Fig. S11 ^{1}H NMR (400 MHz, Chloroform-*d*)

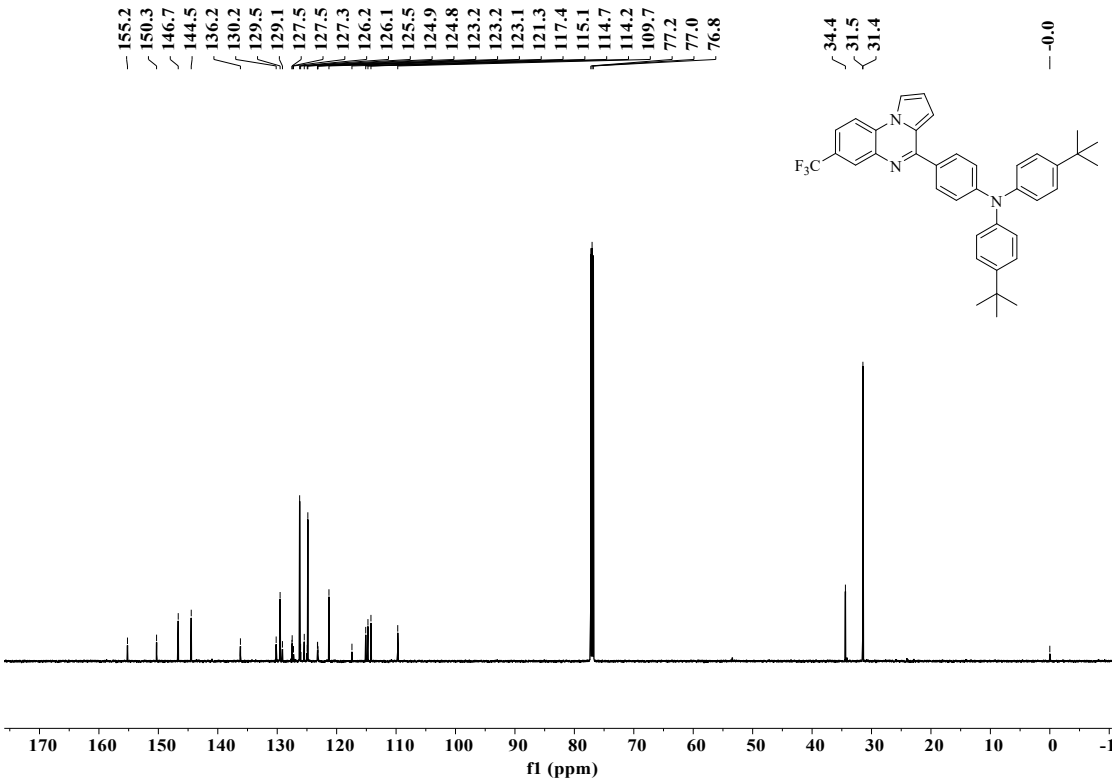


Fig. S12 ^{13}C NMR (100 MHz, Chloroform-*d*)

2. Photophysical properties

2.1 Lippert-Mataga equation

The Lippert-Mataga equation is used to determine the relationship between the Stokes displacement $\Delta\nu_{ST}$ and different solvent polarities, which fits the Stokes displacement and oriented dipoles curves of molecules in solvents of different polarities, and is used to estimate the variation (μ_{CT} - μ_g) in dipole moment between the ground and excited states.

$$\Delta\nu_{ST} = \Delta\nu_{ST}^{0} + \left[\frac{2}{4\pi\varepsilon_0 hca^3}\right] \times (\mu_{CT} - \mu_g)^2 \times \Delta f(\varepsilon,n)$$

$\Delta\nu_{ST}$ is the Stokes shift; (μ_{CT} - μ_g) is the dipole moment variation between the excited and ground states; ε_0 is the vacuum permittivity; h is the Planck's constant; c is the celerity of light; a is the value of the Onsager cavity radius; $\Delta f(\varepsilon,n)$ defined by:

$$\Delta f(\varepsilon,n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n2 - 1}{2n2 + 1}$$

ε is the solvent dielectric constant; n is the solvent refractive index.

In addition, the ground state dipole moments μ_g of compounds **CH_3-PQ-TPA**, **PQ-TPA** and **CF_3-PQ-TPA** were calculated by DFT calculations, which were 0.609 D, 1.135 D and 4.537 D, respectively.

Table S1. Detailed absorption and emission peak positions of **CH_3-PQ-TPA** in different solvents.

Solvents	ε	n	$\Delta f(\varepsilon,n)$	λ_{ex} (nm)	λ_{em} (nm)	ν_a (cm^{-1})	ν_f (cm^{-1})	ν_a-ν_f (cm^{-1})
n-Hexane	1.9	1.375	0.0012	376	433	26596	23095	3501
Toluene	2.38	1.494	0.014	378	461	26455	21692	4763
Ethyl acetate	6.02	1.372	0.2	373	483	26810	20704	6106
Dichloromethane	8.93	1.424	0.217	378	507	26455	19724	6731
Dimethyl formamide	37	1.427	0.276	375	520	26667	19231	7436
Dimethyl sulfoxide	48.9	1.48	0.264	380	528	26316	18939	7376
Triethylamine	2.42	1.401	0.048	376	450	26596	22222	4374
Butyl ether	3.08	1.399	0.096	376	433	26596	23095	3501
Isopropyl ether	3.88	1.368	0.145	374	458	26738	21834	4904

Table S2. Detailed absorption and emission peak positions of **PQ-TPA** in different solvents.

Solvents	ε	n	$\Delta f(\varepsilon,n)$	λ_{ex} (nm)	λ_{em} (nm)	ν_a (cm^{-1})	ν_f (cm^{-1})	ν_a-ν_f (cm^{-1})
n-Hexane	1.9	1.375	0.0012	375	435	26667	22989	3678
Toluene	2.38	1.494	0.014	377	461	26525	21692	4833
Ethyl acetate	6.02	1.372	0.2	371	487	26954	20534	6420
Dichloromethane	8.93	1.424	0.217	377	511	26525	19569	6956
Dimethyl formamide	37	1.427	0.276	373	526	26810	19011	7798
Dimethyl sulfoxide	48.9	1.48	0.264	378	531	26455	18832	7623
Triethylamine	2.42	1.401	0.048	375	451	26667	22173	4494
Butyl ether	3.08	1.399	0.096	375	452	26667	22124	4543
Isopropyl ether	3.88	1.368	0.145	374	460	26738	21739	4999

Table S3. Detailed absorption and emission peak positions of **CF_3-PQ-TPA** in different solvents.

Solvents	ε	n	$\Delta f(\varepsilon,n)$	λ_{ex} (nm)	λ_{em} (nm)	ν_a (cm^{-1})	ν_f (cm^{-1})	ν_a-ν_f (cm^{-1})
n-Hexane	1.9	1.375	0.0012	390	451	25641	22173	3468
Toluene	2.38	1.494	0.014	390	478	25641.	20921	4721
Ethyl acetate	6.02	1.372	0.2	383	513	26110	19493	6616
Dichloromethane	8.93	1.424	0.217	388	533	25773	18762	7011
Dimethyl formamide	37	1.427	0.276	384	555	26042	18018	8024
Dimethyl sulfoxide	48.9	1.48	0.264	388	561	25773	17825	7948
Triethylamine	2.42	1.401	0.048	389	470	25707	21277	4430
Butyl ether	3.08	1.399	0.096	390	467	25641	21413	4228
Isopropyl ether	3.88	1.368	0.145	389	480	25707	20833	4874

2.2 Oxidative titration fluorescence spectroscopy

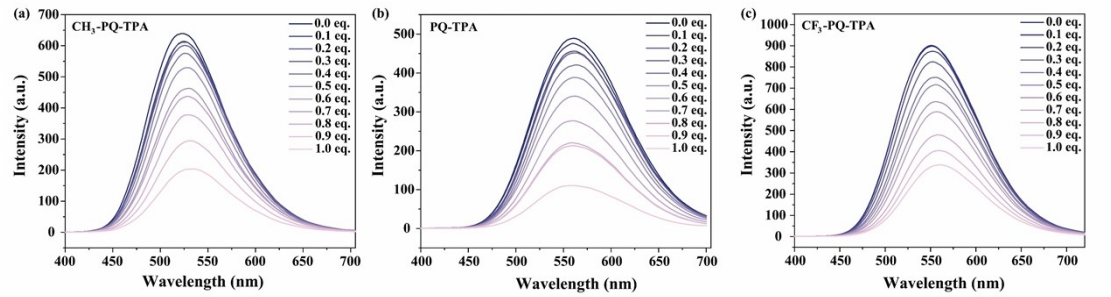


Fig. S13. (a) Photoluminescence spectra recorded upon oxidation of **CH_3-PQ-TPA** and (b) **PQ-TPA** and (c) **CF_3-PQ-TPA** by $Cu(ClO_4)_2$ in DCM/ACN (1:1,V/V) solvent.

3. Electrochemical properties

3.1 Cyclic voltammetry of compound 3a, 3b and 3c

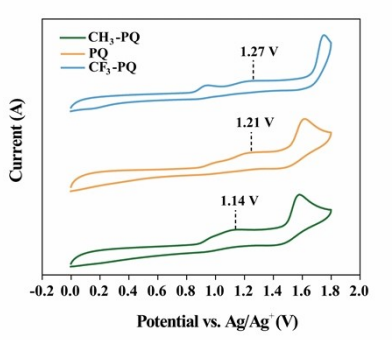


Fig. S14. (a) Cyclic voltammetry of compound **3a**,**3b** and **3c** (1×10^{-3} M) in DCM/ACN (1:1,V/V) solvent and 0.1 M Bu_4NPF_6 are referenced to the Ag/Ag^+ couple. Scan rate: 100 $mV \cdot s^{-1}$.

3.2 Electron transfer constants

The electron transfer constant of the molecule during the redox process can be calculated from the measured cyclic voltammetry curve according to the Nicholson method.

According to the Randles-Sevcik equation:

$$i_p = 2.69\times10^5 A D_0^{1/2} v^{1/2} c^* = R v^{1/2}$$

i_p is the peak current, A; A is the electrode area, cm^2; D_0 is the diffusion velocity, $cm^2 \bullet s^{-1}$; v is the scanning velocity, $V \bullet s^{-1}$; c^* is the concentration, $mol \bullet cm^{-3}$. R is the slope of the fitted curve corresponding to different peak currents at different scan rates, and is a constant.

According to the relationship between the dimensionless constant ψ and the peak voltage difference ΔE_p:

$$\psi = (-0.6288+0.0021\Delta E_p)/(1-0.017\Delta E_p)$$

Bringing ψ and R into Nicholson's formula:

$$k_{ET} = \psi\left(\frac{\pi D 0 F v}{RT}\right)^{1/2} = 184\,\psi R$$

k_{ET} is the electron transfer rate constant; F is the Faraday constant, $C \bullet mol^{-1}$; T is the temperature,°C.

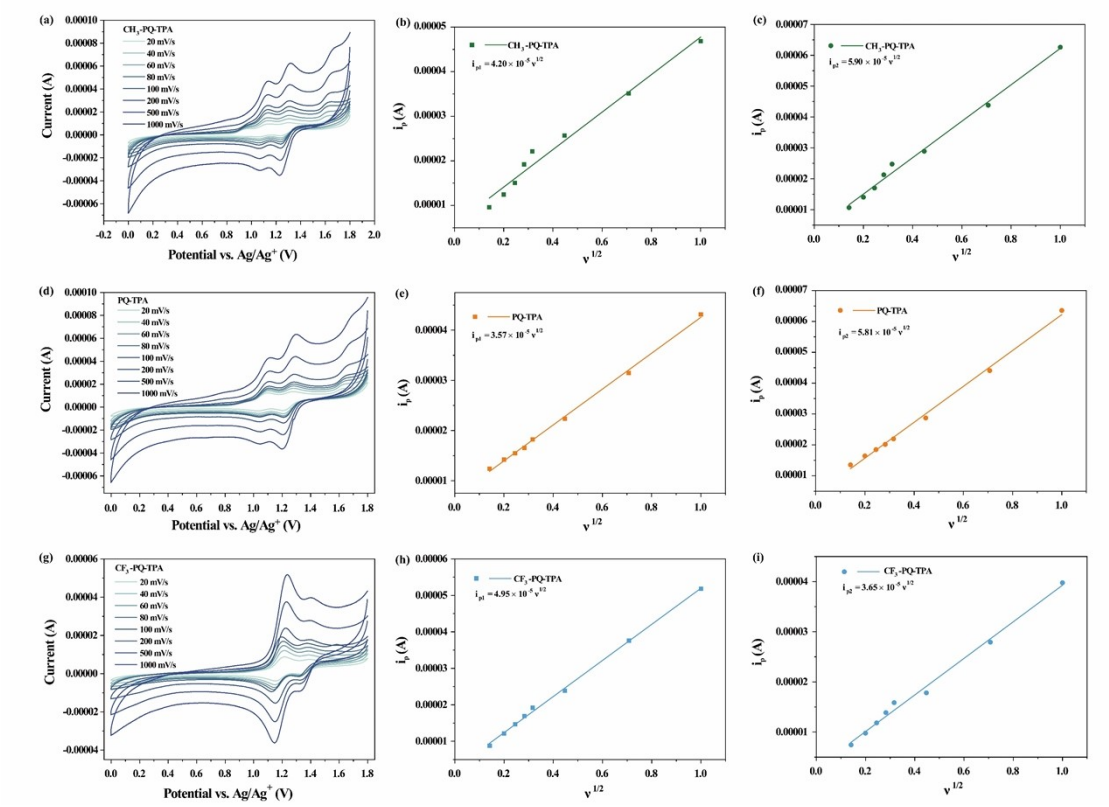


Fig. S15 Cyclic voltammetry at different scanning rate and evaluation of electron-transfer constant.

Table. S4 Electron transfer constants k_{ET} and related data for **CH_3-PQ-TPA**, **PQ-TPA** and **CF_3-PQ-TPA.**

Compound	R_1	ΔE_{P1}(V)	ψ_1	R_2	ΔE_{P2}(V)	ψ_2	k_{ET1}	k_{ET2}
CH_3-PQ-TPA	4.20×10^{-5}	7.55×10^{-2}	1.66	5.90×10^{-5}	8.03×10^{-2}	1.26	0.013	0.014
PQ-TPA	3.57×10^{-5}	7.03×10^{-2}	2.46	5.81×10^{-5}	7.18×10^{-2}	2.18	0.016	0.023
CF_3-PQ-TPA	4.95×10^{-5}	7.57×10^{-2}	1.64	3.65×10^{-5}	7.01×10^{-2}	2.52	0.015	0.017

3.3 Fabrication of the electrochromic device

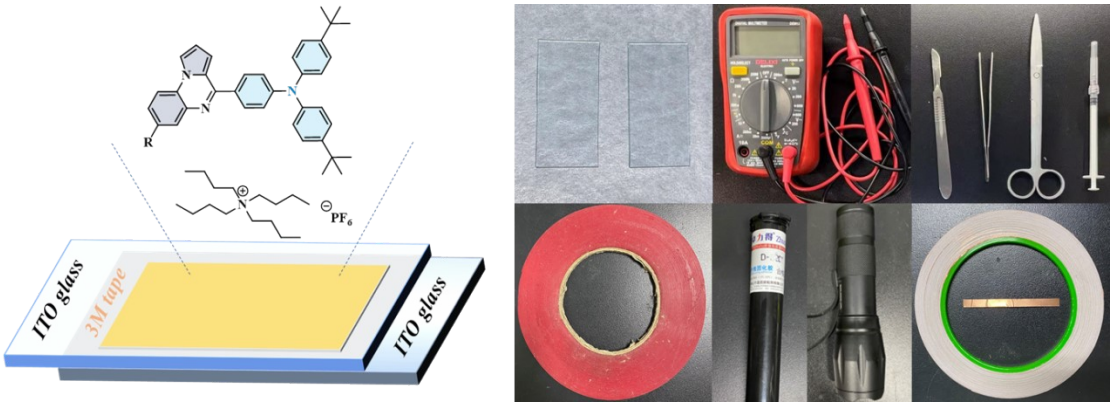


Fig. S16. Device architectures schema and tools.

3.4 Stability of electrochromic switching response in ECDs

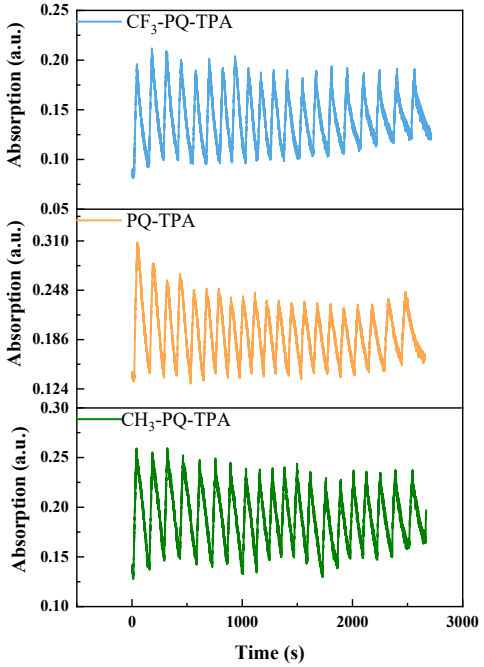


Fig. S17. Cyclic stability of electrochromic devices.

3.5 Coloration efficiency

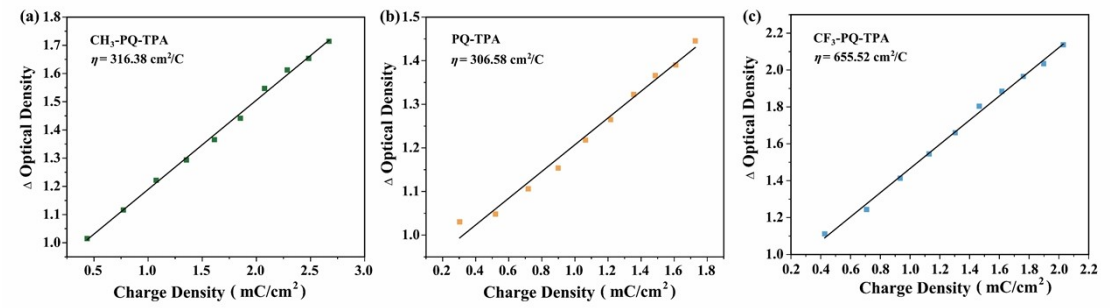


Fig. S18. Optical density versus charge density curve for ECD.

3.6 Switching times and electrochemical cyclic stability

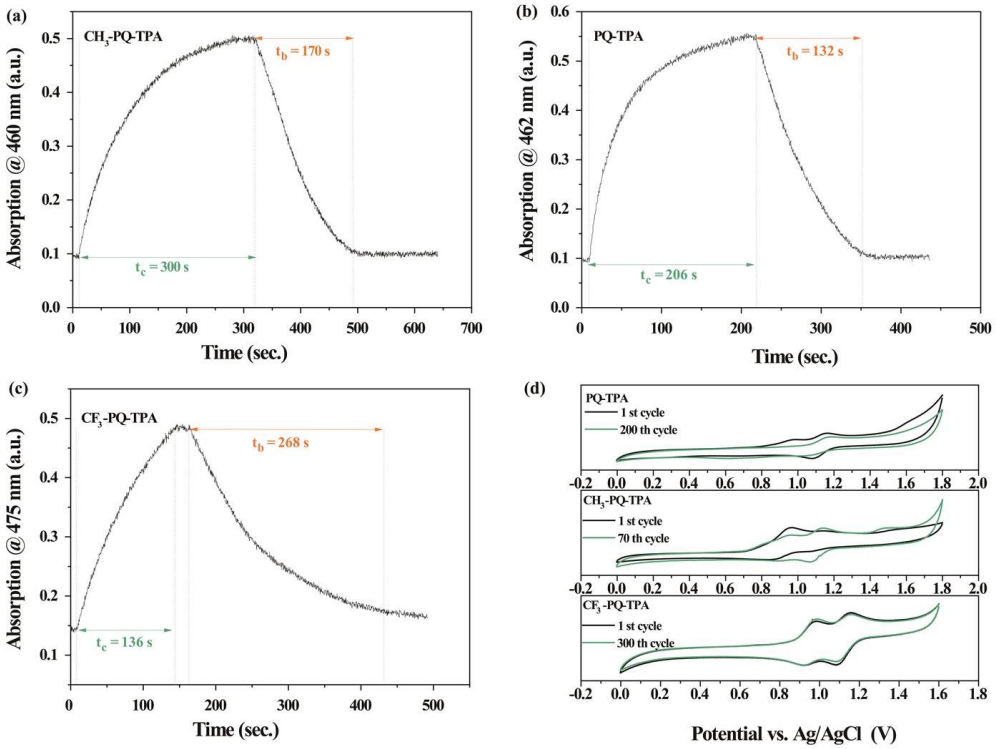


Fig. S19. Switching times and cyclic stability of electrochromic devices.

4. Crystal structure data

Table.S5 Crystal data and structure refinement for compound **CH_3-PQ-TPA** (CCDC: 2270406).

Empirical formula	$C_{38}H_{39}N_3$
Formula weight	537.72
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P21
a/Å	5.85735(15)
b/Å	11.2386(3)
c/Å	23.0899(6)
α/°	90
β/°	90.4439(9)
γ/°	90
Volume/Å^3	1519.93(7)
Z	2
ρcalcg/cm^3	1.175
μ/mm^{-1}	0.521
F(000)	576.0
Crystal size/mm^3	0.1 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.658 to 153.678

Index ranges	$-7 \le h \le 7, -13 \le k \le 12, -28 \le l \le 28$
Reflections collected	52046
Independent reflections	5819 [R_{int} = 0.0555, R_{sigma} = 0.0221]
Data/restraints/parameters	5819/117/418
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0357, wR_2 = 0.0822
Final R indexes [all data]	R_1 = 0.0370, wR_2 = 0.0831

Table.S6 Crystal data and structure refinement for compound **PQ-TPA** (CCDC: 2270406).

Empirical formula	$C_{37}H_{37}N_3$
Formula weight	523.69
Temperature/K	273.15
Crystal system	triclinic
Space group	P-1
a/Å	9.533(7)
b/Å	10.637(7)
c/Å	15.514(10)
α/°	72.169(18)
β/°	86.418(19)
γ/°	83.43(2)
Volume/Å^3	1487.1(17)
Z	2
ρcalcg/cm^3	1.170
μ/mm^{-1}	0.068
F(000)	560.0
Crystal size/mm^3	0.15 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.042 to 50.038
Index ranges	$-11 \le h \le 11, -12 \le k \le 12, -18 \le l \le 18$
Reflections collected	30997
Independent reflections	5252 [R_{int} = 0.0875, R_{sigma} = 0.0645]
Data/restraints/parameters	5252/0/368
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0530, wR_2 = 0.1397
Final R indexes [all data]	R_1 = 0.0808, wR_2 = 0.1628

Table.S7 Crystal data and structure refinement for compound **CF_3-PQ-TPA** (CCDC: 2412717).

Empirical formula	$C_{38}H_{36}F_3N_3$
Formula weight	591.70
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	16.10910(10)
b/Å	17.5255(2)
c/Å	35.0880(4)
α/°	79.4790(10)
β/°	79.6190(10)
γ/°	79.8640(10)
Volume/$Å^3$	9474.65(17)
Z	12
ρcalcg/cm^3	1.244
μ/mm^{-1}	0.691
F(000)	3744.0
Crystal size/mm^3	0.15 × 0.13 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.186 to 148.2
Index ranges	$-20 \le h \le 18$, $-21 \le k \le 21$, $-43 \le l \le 43$
Reflections collected	112254
Independent reflections	37030 [R_{int} = 0.0346, R_{sigma} = 0.0423]
Data/restraints/parameters	37030/1480/2918
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0521, wR_2 = 0.1394
Final R indexes [all data]	R_1 = 0.0703, wR_2 = 0.1535

5. Cartesian coordination of all the optimized structures

CH_3-PQ-TPA

Zero-point correction= 0.675596 (Hartree/Particle)

Thermal correction to Energy= 0.712773

Thermal correction to Enthalpy= 0.713717

Thermal correction to Gibbs Free Energy= 0.602841

Sum of electronic and zero-point Energies= -1635.208669

Sum of electronic and thermal Energies= -1635.171492

Sum of electronic and thermal Enthalpies= -1635.170548

Sum of electronic and thermal Free Energies= -1635.281424

Cartesian coordinates

C	-8.61662200	0.69092600	0.06433000
C	-7.90601800	1.90656700	-0.01589500
C	-6.51946800	1.85324300	-0.05942200
C	-5.81485300	0.63188200	-0.03029600
C	-6.56018700	-0.56851100	0.04333700
C	-7.95973500	-0.53015200	0.09426000
N	-4.43509200	0.66766300	-0.04960800
C	-3.76364500	-0.46083200	-0.00966800
C	-4.42168300	-1.74292600	-0.00021100
N	-5.82652600	-1.75848300	0.04488400
C	-2.28504900	-0.36247200	-0.00046500
C	-1.46365700	-1.26406000	0.69587800
C	-0.08127000	-1.11661800	0.71193800
C	0.53598900	-0.06611600	0.01135800

C	-0.28302100	0.84557600	-0.68145800
C	-1.66280300	0.70394900	-0.67204900
N	1.94248400	0.07470300	0.00739700
C	2.53654100	1.36896700	0.01025000
C	2.78413200	-1.07303500	0.00085200
C	3.92187800	-1.12980600	0.82040600
C	4.75108000	-2.24546800	0.79826900
C	4.48553000	-3.35817900	-0.01871400
C	3.34116700	-3.28759600	-0.82465500
C	2.50930500	-2.16796200	-0.82719500
C	3.61607800	1.66149400	-0.83682300
C	4.20411000	2.92111900	-0.81850600
C	3.74208300	3.94882800	0.02216900
C	2.65779800	3.64151700	0.85519500
C	2.06879000	2.37695900	0.86133000
C	-4.00130300	-3.07083900	-0.07192200
C	-5.15266000	-3.88307000	-0.05425100
C	-6.26147700	-3.05726400	0.01886700
H	-5.92523300	2.76028600	-0.11370700
H	-8.53270600	-1.44896300	0.15695800
H	-1.91112100	-2.06255300	1.27713700
H	0.52859000	-1.81065500	1.27951200
H	0.17302300	1.66183200	-1.23075000
H	-2.28726100	1.41461000	-1.20209600
H	4.15257500	-0.29378200	1.47234200
H	5.62123100	-2.24871100	1.44836800
H	3.08582200	-4.10981400	-1.48329500
H	1.63977000	-2.14326800	-1.47571700
H	3.99129500	0.89515000	-1.50710100
H	5.03771000	3.10674900	-1.48953300

H	2.26029500	4.38931900	1.53177600
H	1.23882800	2.17066300	1.52919100
H	-2.97901000	-3.40373700	-0.15415800
H	-5.18170400	-4.96281600	-0.09702900
H	-7.31134400	-3.30113100	0.03758200
C	4.42248800	5.32916600	-0.00176400
C	4.31632700	5.93233600	-1.42273700
C	3.77559600	6.31659700	0.98739600
C	5.91456700	5.17577200	0.37765400
H	4.79367100	5.29475800	-2.17267300
H	3.26934500	6.06403500	-1.71457400
H	4.80545400	6.91232200	-1.45892300
H	3.84785600	5.96363600	2.02131700
H	4.28796500	7.28250300	0.93259600
H	2.71929100	6.49042800	0.75784600
H	6.41605700	6.15009100	0.35759900
H	6.02126100	4.75902200	1.38445600
H	6.44484600	4.51495400	-0.31433600
C	5.43083200	-4.57225400	-0.00104500
C	5.48980200	-5.16027200	1.42892100
C	4.96789400	-5.68612600	-0.95888700
C	6.84949800	-4.12674700	-0.42858200
H	5.84953400	-4.42652400	2.15624300
H	4.49991500	-5.49544100	1.75525300
H	6.16776000	-6.02074900	1.46122600
H	4.93558700	-5.34313100	-1.99820500
H	5.66621700	-6.52790100	-0.91123300
H	3.97586800	-6.06556600	-0.69289400
H	7.53862300	-4.97885200	-0.41652000
H	6.84042800	-3.71159200	-1.44167800

H	7.25412300	-3.36217000	0.24110000
C	-8.64552200	3.22308600	-0.04793500
H	-7.95314400	4.06647800	-0.11012800
H	-9.25848500	3.35884200	0.85066900
H	-9.70258800	0.70799200	0.10409200
H	-9.32148200	3.28042100	-0.90901600

PQ-TPA

Zero-point correction= 0.648318 (Hartree/Particle)

Thermal correction to Energy= 0.683549

Thermal correction to Enthalpy= 0.684493

Thermal correction to Gibbs Free Energy= 0.578283

Sum of electronic and zero-point Energies= -1595.915399

Sum of electronic and thermal Energies= -1595.880168

Sum of electronic and thermal Enthalpies= -1595.879224

Sum of electronic and thermal Free Energies= -1595.985433

Cartesian coordinates

C	-8.78873800	1.42496700	0.08541800
C	-7.98242300	2.57123600	0.00948100
C	-6.60392800	2.44429700	-0.04256200
C	-5.98816300	1.17617300	-0.02529100
C	-6.82057500	0.03097500	0.04393300
C	-8.21423500	0.16041100	0.10317700
N	-4.60949600	1.11241400	-0.04986900
C	-4.02066800	-0.06118300	-0.01964500
C	-4.76978000	-1.29252200	-0.01750900
N	-6.17209200	-1.20771100	0.03315500

C	-2.53907800	-0.07085000	-0.01300800
C	-1.78607100	-1.03302700	0.67958100
C	-0.39671700	-0.98775100	0.69526700
C	0.29586400	0.01696400	-0.00221700
C	-0.45416000	0.98855400	-0.69202300
C	-1.84066000	0.94923700	-0.68167100
N	1.70891200	0.05337600	-0.00610400
C	2.39834600	1.29924000	0.00363300
C	2.46069500	-1.15555600	-0.01018800
C	3.58184900	-1.30428100	0.82034600
C	4.31761900	-2.48393200	0.80554500
C	3.97073100	-3.57098600	-0.01529000
C	2.84648500	-3.40614000	-0.83556500
C	2.10867100	-2.22251600	-0.84532500
C	3.50871600	1.50778300	-0.82839900
C	4.18622300	2.72159500	-0.80709400
C	3.78818000	3.78487700	0.02175800
C	2.67421300	3.56076900	0.84187600
C	1.99502200	2.34233500	0.84541900
C	-4.44564500	-2.64575700	-0.10200300
C	-5.65227400	-3.37416700	-0.08637800
C	-6.69870700	-2.47244200	-0.00183100
H	-8.43923500	3.55588500	-0.00420400
H	-5.95244600	3.31036800	-0.09337300
H	-8.84498900	-0.71977400	0.16275100
H	-2.29099900	-1.79834600	1.25835500
H	0.16067500	-1.72648200	1.26025000
H	0.06059000	1.77048900	-1.23921100
H	-2.41128000	1.70573100	-1.20899400
H	3.87220000	-0.49053500	1.47666900

H	5.17727600	-2.55889700	1.46505600
H	2.53363100	-4.20456400	-1.49842400
H	1.25103300	-2.12586600	-1.50287700
H	3.83665000	0.71319500	-1.49053600
H	5.04030600	2.84264900	-1.46689500
H	2.32352700	4.33911700	1.50961000
H	1.14352800	2.20036100	1.50272900
H	-3.44986900	-3.04973400	-0.19085200
H	-5.75839400	-4.44866600	-0.13818900
H	-7.76306500	-2.64155800	0.01900400
C	4.56191600	5.11508900	-0.00376400
C	4.50230400	5.71762500	-1.42775500
C	3.97998500	6.14881300	0.97889500
C	6.03890700	4.86287200	0.38224500
H	4.94054000	5.04672300	-2.17253800
H	3.46752200	5.91576400	-1.72537300
H	5.05445700	6.66353900	-1.46582000
H	4.01974400	5.79454700	2.01417800
H	4.56014800	7.07562500	0.92542200
H	2.94031500	6.39682300	0.74169500
H	6.60518000	5.80074700	0.35762000
H	6.11407200	4.44677000	1.39215700
H	6.52556600	4.16307800	-0.30349000
C	4.80546300	-4.86334800	0.01975400
C	4.77028000	-5.45884000	1.44749800
C	4.27409400	-5.92879900	-0.95783000
C	6.27017700	-4.54549000	-0.36455900
H	5.17505900	-4.76317300	2.18848100
H	3.74494300	-5.70238100	1.74418200
H	5.36522700	-6.37810700	1.49354600

H	4.29739500	-5.57843300	-1.99495600
H	4.89761200	-6.82668000	-0.89926100
H	3.24723200	-6.22495400	-0.71982400
H	6.87983500	-5.45554100	-0.33220400
H	6.32867200	-4.13327900	-1.37718400
H	6.72172500	-3.81901100	0.31746700
H	-9.86915200	1.52066900	0.13124200

CF_3-PQ-TPA

Zero-point correction= 0.653176 (Hartree/Particle)

Thermal correction to Energy= 0.692038

Thermal correction to Enthalpy= 0.692982

Thermal correction to Gibbs Free Energy= 0.577680

Sum of electronic and zero-point Energies= -1932.946626

Sum of electronic and thermal Energies= -1932.907764

Sum of electronic and thermal Enthalpies= -1932.906820

Sum of electronic and thermal Free Energies= -1933.022122

Cartesian coordinates

C	7.92646400	-0.61324200	-0.12901800
C	7.35709800	0.66756200	-0.03168900
C	5.97995800	0.81611100	0.02901700
C	5.12966400	-0.30550000	0.00110900
C	5.72136000	-1.59094700	-0.08710900
C	7.11354600	-1.73563900	-0.15799900
N	3.76745800	-0.09526400	0.03215300
C	2.95733100	-1.12957400	-0.00467400
C	3.45117800	-2.48414600	-0.02172000
N	4.84428000	-2.67600000	-0.08517700
C	1.50493500	-0.84554600	-0.00337500

C	0.56947600	-1.64343100	-0.68319900
C	-0.78245700	-1.32185000	-0.69194200
C	-1.25560500	-0.19108200	-0.00279100
C	-0.32080500	0.61649100	0.67415800
C	1.02885200	0.29969700	0.65907600
N	-2.62963800	0.13120700	0.00410100
C	-3.05112400	1.49243400	-0.00528000
C	-3.61406300	-0.89785400	0.01062800
C	-4.74155000	-0.81493700	-0.82030700
C	-5.70938200	-1.81288400	-0.79527600
C	-5.59777400	-2.94134900	0.03543100
C	-4.46118000	-3.01150900	0.85236100
C	-3.49130700	-2.00914400	0.85287200
C	-4.08367000	1.92693300	0.83908400
C	-4.50326400	3.25231200	0.81292700
C	-3.91170500	4.20635100	-0.03337100
C	-2.87587100	3.75591600	-0.86290700
C	-2.45623400	2.42574700	-0.86153200
C	2.87049400	-3.74771800	0.05584100
C	3.91113300	-4.69911300	0.02243800
C	5.11283200	-4.02058300	-0.06524400
H	5.51914000	1.79491700	0.08967000
H	7.56046600	-2.71994900	-0.23901400
H	0.90619100	-2.49702800	-1.26058300
H	-1.47959000	-1.93901200	-1.24752900
H	-0.66454000	1.49095600	1.21522500
H	1.74190600	0.93087600	1.17766100
H	-4.85514300	0.03689400	-1.48263300
H	-6.56737200	-1.71031100	-1.45316600
H	-4.32164900	-3.85256400	1.52168100

H	-2.63234800	-2.08904800	1.51102700
H	-4.55548600	1.21968600	1.51328700
H	-5.30531900	3.54841800	1.48280600
H	-2.38331800	4.44160400	-1.54253700
H	-1.66016200	2.10999600	-1.52788500
H	1.81607900	-3.95075600	0.15241000
H	3.80417500	-5.77383300	0.06498400
H	6.12291500	-4.39562200	-0.09684100
C	-4.40664100	5.66351700	-0.02180300
C	-4.22783100	6.25864300	1.39513000
C	-3.63332000	6.55026300	-1.01582300
C	-5.90497900	5.70120900	-0.40617700
H	-4.78645400	5.69418100	2.14754400
H	-3.17358700	6.25583800	1.69048200
H	-4.58569900	7.29401000	1.42216600
H	-3.74461500	6.19953000	-2.04703100
H	-4.01757200	7.57441600	-0.97279900
H	-2.56463200	6.58920000	-0.78108500
H	-6.27537500	6.73252800	-0.39971400
H	-6.06234500	5.29037600	-1.40882200
H	-6.51846100	5.12322400	0.29129600
C	-6.69352700	-4.02202300	0.02206500
C	-6.82118100	-4.61173400	-1.40272900
C	-6.38682500	-5.17751100	0.99294700
C	-8.04423800	-3.39105900	0.43609600
H	-7.08281600	-3.84598500	-2.13900100
H	-5.88087100	-5.07345500	-1.72109600
H	-7.60302300	-5.37920100	-1.42939800
H	-6.31652200	-4.83194500	2.02949400
H	-7.19020000	-5.91964100	0.94726300

H	-5.45199700	-5.68736700	0.73798800
H	-8.83776300	-4.14691200	0.42735500
H	-7.98639500	-2.97063600	1.44536200
H	-8.34344200	-2.58736900	-0.24318500
C	8.25258500	1.87145100	0.06399900
H	9.00321600	-0.72232500	-0.19054000
F	9.39077700	1.70667500	-0.64999500
F	8.62969200	2.11551600	1.34230700
F	7.64883000	2.99215900	-0.38671900

CH_3-PQ-TPA$^{\bullet+}$

Zero-point correction= 0.676271 (Hartree/Particle)

Thermal correction to Energy= 0.713301

Thermal correction to Enthalpy= 0.714245

Thermal correction to Gibbs Free Energy= 0.604046

Sum of electronic and zero-point Energies= -1634.992319

Sum of electronic and thermal Energies= -1634.955289

Sum of electronic and thermal Enthalpies= -1634.954345

Sum of electronic and thermal Free Energies= -1635.064543

Cartesian coordinates

C	-8.54580000	0.73192600	0.12024400
C	-7.82005700	1.93312500	-0.07236700
C	-6.44276900	1.84910000	-0.17567300
C	-5.76299300	0.60974500	-0.09878200
C	-6.52669800	-0.57737700	0.08458800
C	-7.92012700	-0.50238600	0.19835900
N	-4.39849800	0.60900700	-0.17980800

C	-3.73998600	-0.53473200	-0.08003600
C	-4.41428600	-1.79690800	0.01352000
N	-5.81819600	-1.77487200	0.11723000
C	-2.27251500	-0.41746800	-0.05845700
C	-1.44147800	-1.34577200	0.60486200
C	-0.06755000	-1.19126500	0.62402500
C	0.53466400	-0.08744800	-0.02349900
C	-0.29273000	0.86176800	-0.67018600
C	-1.66249600	0.69751600	-0.67779600
N	1.92433000	0.06894300	-0.01007000
C	2.50495900	1.36617700	0.00677800
C	2.77886200	-1.06573700	-0.01325500
C	3.92593400	-1.08938400	0.80071400
C	4.75862800	-2.19706400	0.78508300
C	4.50115400	-3.31637100	-0.03372800
C	3.35229500	-3.26676000	-0.84133000
C	2.50072700	-2.16702300	-0.83818800
C	3.62442100	1.64944700	-0.79608100
C	4.18865200	2.91512200	-0.76879700
C	3.68031000	3.94391700	0.05111500
C	2.56540300	3.63412500	0.84857000
C	1.98099500	2.37201300	0.83351800
C	-4.03062500	-3.13915300	-0.01157900
C	-5.19882800	-3.91982300	0.09764900
C	-6.28227900	-3.06486000	0.17668200
H	-5.83353500	2.73641700	-0.31363900
H	-8.51267200	-1.39794900	0.34522900
H	-1.88524200	-2.16413200	1.15864700
H	0.55021600	-1.88970800	1.17612100
H	0.15747500	1.69991500	-1.18885600

H	-2.29736200	1.41584700	-1.18198200
H	4.14195200	-0.25065200	1.45318100
H	5.62725000	-2.19478400	1.43472300
H	3.11704900	-4.09171000	-1.50225800
H	1.63741200	-2.14630900	-1.49443000
H	4.02708200	0.88365200	-1.44985500
H	5.04117200	3.11051000	-1.41022600
H	2.14576100	4.38225700	1.50955900
H	1.13712300	2.15587700	1.47981400
H	-3.02585200	-3.51092300	-0.13562100
H	-5.25440000	-4.99879100	0.10592800
H	-7.33517000	-3.28336500	0.24999800
C	4.34620500	5.32764400	0.04679700
C	4.29141700	5.91291900	-1.38614200
C	3.64953800	6.31485000	1.00152700
C	5.82353800	5.18157000	0.48744400
H	4.81524700	5.28199800	-2.11000100
H	3.25758800	6.03017300	-1.72610300
H	4.76668000	6.89870500	-1.40268500
H	3.68488100	5.97439700	2.04151600
H	4.15700900	7.28259300	0.95855400
H	2.60310300	6.48286300	0.72672000
H	6.31162300	6.16129300	0.48207700
H	5.89468900	4.77352900	1.50060000
H	6.39031100	4.52696600	-0.18094900
C	5.46186800	-4.51395000	-0.01981200
C	5.53165100	-5.09317800	1.41493200
C	5.01212000	-5.63524300	-0.97490700
C	6.87067300	-4.03778700	-0.45192000
H	5.88991300	-4.35689400	2.14014500

H	4.54988600	-5.44483800	1.74756800
H	6.22097800	-5.94300100	1.43953300
H	4.97587500	-5.29850300	-2.01608700
H	5.72426700	-6.46365900	-0.92518200
H	4.02880100	-6.03393500	-0.70475800
H	7.56751200	-4.88181000	-0.44440100
H	6.85397300	-3.62234000	-1.46447500
H	7.27063000	-3.27315000	0.22023300
C	-8.54612500	3.25249900	-0.15345700
H	-7.85154500	4.08191600	-0.30395900
H	-9.11239000	3.44844800	0.76371900
H	-9.62758500	0.77696700	0.20935900
H	-9.26317200	3.25793900	-0.98171800

PQ-TPA$^{\bullet+}$

Zero-point correction= 0.648998 (Hartree/Particle)

Thermal correction to Energy= 0.684123

Thermal correction to Enthalpy= 0.685067

Thermal correction to Gibbs Free Energy= 0.579283

Sum of electronic and zero-point Energies= -1595.697703

Sum of electronic and thermal Energies= -1595.662578

Sum of electronic and thermal Enthalpies= -1595.661634

Sum of electronic and thermal Free Energies= -1595.767419

Cartesian coordinates

C	-8.71353000	1.46574000	0.10562900
C	-7.89139100	2.59433400	-0.07397300
C	-6.52327900	2.43840600	-0.17507600
C	-5.93448200	1.15359800	-0.10552000

C	-6.78515900	0.02379100	0.06602900
C	-8.17077300	0.18950000	0.17607800
N	-4.57197600	1.05527700	-0.18197100
C	-3.99926400	-0.13258400	-0.08773600
C	-4.76269100	-1.34372700	-0.00330700
N	-6.16237900	-1.22208500	0.09304900
C	-2.52598400	-0.12306200	-0.06405500
C	-1.76772700	-1.10785000	0.60416400
C	-0.38586200	-1.05576200	0.62466900
C	0.29639700	-0.00265500	-0.02715700
C	-0.45661300	1.00278300	-0.67900300
C	-1.83517100	0.94110200	-0.68707800
N	1.69524000	0.04904300	-0.01339900
C	2.37110300	1.29801300	0.00596400
C	2.45913800	-1.14795000	-0.01790200
C	3.60133400	-1.26168300	0.79575800
C	4.33950400	-2.43442400	0.78545200
C	3.98998300	-3.53259300	-0.02797800
C	2.85110600	-3.39079900	-0.83903100
C	2.09283900	-2.22508000	-0.84073300
C	3.51790900	1.49295800	-0.78537700
C	4.17162300	2.71454900	-0.76056700
C	3.72957900	3.78413700	0.04574300
C	2.58745700	3.56158800	0.83407500
C	1.91333400	2.34537000	0.82129300
C	-4.47498400	-2.70903200	-0.03490000
C	-5.69633700	-3.40527200	0.06226600
C	-6.71679000	-2.47597700	0.14087800
H	-8.33484300	3.58275000	-0.12761900
H	-5.85787700	3.28503400	-0.30365900

H	-8.82052000	-0.66679900	0.31424400
H	-2.27235300	-1.88905500	1.15943900
H	0.17782200	-1.79567700	1.18051900
H	0.05538700	1.80232500	-1.20123100
H	-2.41466100	1.70263800	-1.19458500
H	3.88469500	-0.44170300	1.44630300
H	5.20465900	-2.50188900	1.43603900
H	2.55027500	-4.19638500	-1.49698200
H	1.23437400	-2.13533900	-1.49743600
H	3.87041700	0.69578700	-1.43049700
H	5.04269900	2.84324900	-1.39368800
H	2.21739300	4.34344300	1.48538800
H	1.04962200	2.19551200	1.45994000
H	-3.49816100	-3.15013400	-0.15497000
H	-5.82866500	-4.47757500	0.06304300
H	-7.78282400	-2.62066600	0.20656500
C	4.48992300	5.11806000	0.03465800
C	4.48184300	5.69299100	-1.40360900
C	3.85897300	6.15958200	0.97764500
C	5.95186000	4.87424600	0.48388100
H	4.96593600	5.02207700	-2.11915700
H	3.45993700	5.87626600	-1.75026400
H	5.02223400	6.64453900	-1.42558900
H	3.86291600	5.82558800	2.02034300
H	4.43475700	7.08807800	0.93143300
H	2.82916100	6.40001500	0.69404200
H	6.50605000	5.81791200	0.47155200
H	5.99073400	4.47246500	1.50127800
H	6.47514500	4.17576800	-0.17546400
C	4.83943000	-4.81107200	0.00189600

C	4.82864300	-5.38994500	1.43862800
C	4.30798800	-5.88950000	-0.96099100
C	6.29388300	-4.46698300	-0.40381100
H	5.24244500	-4.68846400	2.16880100
H	3.81206000	-5.64525600	1.75402900
H	5.43321400	-6.30155600	1.47644700
H	4.31592400	-5.55080200	-2.00216900
H	4.94566300	-6.77586600	-0.90216900
H	3.29037700	-6.20282800	-0.70578600
H	6.91118400	-5.37029200	-0.37555500
H	6.33549900	-4.06105100	-1.41948000
H	6.74852900	-3.73587300	0.27099100
H	-9.78827000	1.58933700	0.19073800

CF_3-PQ-TPQ$^{\bullet+}$

Zero-point correction= 0.653870 (Hartree/Particle)

Thermal correction to Energy= 0.692586

Thermal correction to Enthalpy= 0.693531

Thermal correction to Gibbs Free Energy= 0.579268

Sum of electronic and zero-point Energies= -1932.724336

Sum of electronic and thermal Energies= -1932.685619

Sum of electronic and thermal Enthalpies= -1932.684675

Sum of electronic and thermal Free Energies= -1932.798938

Cartesian coordinates

C	7.85618300	-0.58650800	-0.18567000
C	7.27133200	0.67622400	0.03630800
C	5.90014000	0.79469300	0.14955600

C	5.07047800	-0.34381200	0.05154200
C	5.67656200	-1.61220800	-0.15906100
C	7.06880000	-1.72167900	-0.28292200
N	3.71387300	-0.16801200	0.14075900
C	2.91826600	-1.21394000	0.02690400
C	3.42267800	-2.55071300	-0.10258100
N	4.81992700	-2.70776000	-0.21461500
C	1.47265400	-0.91025800	0.02934700
C	0.52712500	-1.69860500	-0.65830900
C	-0.81620700	-1.36447800	-0.66133600
C	-1.26121700	-0.21320900	0.02496400
C	-0.31838400	0.59438100	0.70144400
C	1.01869100	0.24948000	0.69556500
N	-2.62184500	0.13288300	0.01991000
C	-3.01246600	1.49524300	-0.01342400
C	-3.61625400	-0.87660500	0.04159200
C	-4.77637700	-0.74804000	-0.74623000
C	-5.74268000	-1.73987600	-0.71439300
C	-5.61167400	-2.88822900	0.09535900
C	-4.44683700	-2.99152200	0.87615700
C	-3.46166200	-2.01144500	0.85587800
C	-4.09968400	1.94144900	0.76240400
C	-4.47381500	3.27439300	0.71939200
C	-3.80363900	4.21495300	-0.09180200
C	-2.72464400	3.74385800	-0.86064100
C	-2.32698500	2.41278300	-0.82760500
C	2.86938500	-3.83035300	-0.10875400
C	3.92686000	-4.75277500	-0.24282200
C	5.11204400	-4.04444900	-0.30752100
H	5.42715300	1.75612800	0.30710500

H	7.53468000	-2.68449700	-0.45592900
H	0.85822500	-2.54901600	-1.24158000
H	-1.52317700	-1.95635600	-1.23096900
H	-0.65443300	1.46561900	1.25151800
H	1.74448000	0.85966600	1.21917500
H	-4.89563900	0.11266700	-1.39479500
H	-6.61744900	-1.62458000	-1.34495200
H	-4.30562800	-3.84386800	1.52877100
H	-2.58837700	-2.10468600	1.49205400
H	-4.62112200	1.24676500	1.41145100
H	-5.30170200	3.59555400	1.34207600
H	-2.18733900	4.42080400	-1.51273500
H	-1.50791900	2.07441700	-1.45261900
H	1.82505400	-4.07230300	0.00929200
H	3.84216600	-5.82932600	-0.27814600
H	6.12681900	-4.39763500	-0.39256200
C	-4.26189400	5.67965000	-0.10790700
C	-4.13490900	6.26416500	1.32119400
C	-3.42115200	6.54560400	-1.06453200
C	-5.74150000	5.74405900	-0.56141400
H	-4.74703500	5.71954300	2.04577400
H	-3.09710100	6.23857500	1.66807000
H	-4.46680500	7.30695000	1.32535600
H	-3.49212500	6.20002000	-2.10099800
H	-3.78706400	7.57570600	-1.03888400
H	-2.36485300	6.56823800	-0.77749300
H	-6.08054500	6.78455300	-0.57208300
H	-5.86419200	5.33872400	-1.57074900
H	-6.40367000	5.18868400	0.10906000
C	-6.71487700	-3.95547300	0.09752700

C	-6.87247300	-4.52296200	-1.33534800
C	-6.39883500	-5.12258600	1.05099500
C	-8.04851100	-3.30663400	0.54395500
H	-7.14998200	-3.74978400	-2.05766500
H	-5.94481700	-4.99077300	-1.67987200
H	-7.65928000	-5.28362900	-1.34749900
H	-6.30391600	-4.79045400	2.08993800
H	-7.21338800	-5.85112900	1.01547000
H	-5.48018000	-5.64701500	0.76851500
H	-8.84369700	-4.05863000	0.54601700
H	-7.96925900	-2.89586500	1.55537900
H	-8.36026500	-2.49971400	-0.12551300
C	8.16729000	1.88027400	0.17970800
H	8.93281200	-0.66854800	-0.28733600
F	9.10520500	1.90673800	-0.79081900
F	8.82154900	1.86088200	1.36090100
F	7.47380300	3.03419300	0.11768300

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