Supplementary Materials

Iodide ion receptors: shape-persistent macrocycles of *syn/anti* configurations

Guang-Wei Zhang, [a] Jia-Yin Xiang, [a] Tao-Tao Zhong, [a] Xin-Ru Zhi, [a] Chuang Gao, [a] Wei Huang, [a] Shuai Yuan, [a] Ling-Hai Xie [a] and Wei Huang [abc*]

[a] *Centre for Molecular Systems and Organic Devices (CMSOD), Key Laboratory for Organic Electronics and Information Displays and Jiangsu Key Laboratory for Biosensors, Institute of Advanced Materials (IAM), Nanjing University of Posts and Telecommunications, 9 Wenyuan Road, Nanjing, 210023, China;* [b] *Frontiers Science Centre for Flexible Electronics (FSCFE), MIIT Key Laboratory of Flexible Electronics (KLOFE), Shaanxi Key Laboratory of Flexible Electronics, Xi'an Key Laboratory of Flexible Electronics, Xi'an Key Laboratory of Biomedical Materials & Engineering, Xi'an Institute of Flexible Electronics, Institute of Flexible Electronics (IFE), Northwestern Polytechnical University, Xi'an 710072, Shaanxi, China;* [c] *Key Laboratory of Flexible Electronics (KLOFE) & Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing 211816, China*

Table of Contents

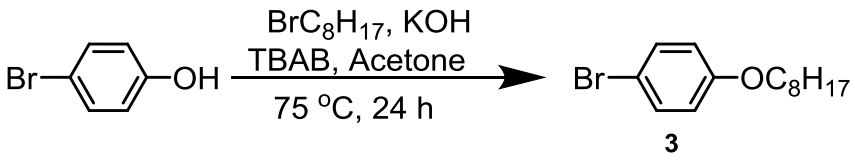
1. General information of synthesis

Chemicals: Unless otherwise stated, all solvents and reagents were purchased from commercial suppliers and used without further purification. All products were separated by column chromatography. Spectrochemical grade solvents were used for optical measurement. Tetrakis(triphenylphosphine)palladium(II) and carbazole were purchased from Aldrich Chemical Co. Boron trifluoride etherate, potassium carbonate, potassium fluoride, and magnesium sulfate were purchased from Sinopharm Holding Chemical Reagent Co Ltd without further purification. Before use, the methylene chloride was dried with anhydrous sodium sulfate. Tetrahydrofuran and toluene were dried over sodium benzophenone anion and distilled under a dry nitrogen atmosphere. Tetrabutylammonium fluoride (TBAF), tetrabutylammonium chloride (TBACl), tetrabutylammonium bromide (TBABr) and tetrabutylammonium iodide (TBAI) were all from Anaiji without purification and used directly.

Characterization: ^{1}H-NMR was recorded on a Bruker 400 MHz spectrometer in d-$CDCl_3$ or d-CD_2Cl_2 with tetramethylsilane (TMS) as the interval standard. For the MALDI-TOF MS spectra, the spectra were recorded in reflective mode, and substrates were used. The best structure of the compound was calculated by Gaussian computer program -Gaussian 09.[1] Absorption spectra were measured with a Shimadzu UV-3150 spectrometer at 25 ℃, and emission spectra were recorded on a Shimadzu RF-530XPC luminescence spectrometer upon excitation at the absorption maxima.

2. General experimental and synthetic details to the ***syn/anti*** **isomers**

2.1 Compound **3**: 1-bromo-4-(octyloxy) benzene



3

Under the protection of nitrogen, bromophenol (275 mmol, 47 g), bromooctane

(261 mmol, 50 g), potassium hydroxide (410 mmol, 23 g) and tetrabutylammonium bromide (4 g) were dissolved in 300 mL of acetone. The reaction was stirred overnight at 75ºC. After cooling to room temperature, undissolved solid was filtered. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography to give pure 1-bromo-4-(octyloxy)benzene (68 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 1H), 6.80 – 6.73 (m, 1H), 3.91 (t, J = 6.6 Hz, 1H), 1.77 (dt, J = 14.6, 6.6 Hz, 1H), 1.50 – 1.24 (m, 6H), 0.94 – 0.82 (m, 3H).

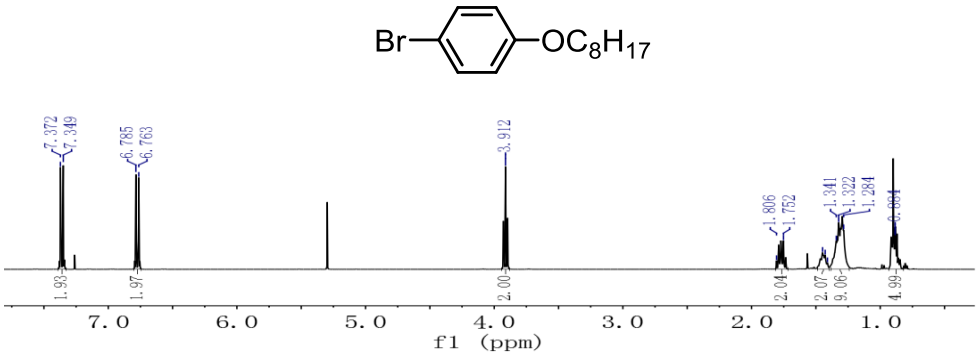
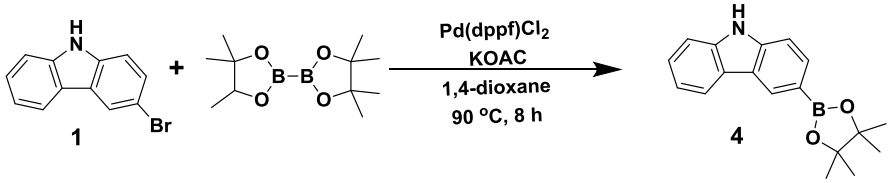


Figure S1. ^{1}H NMR spectrum of **3** recorded in $CDCl_3$

2.2 Compound **4**: 3-(4, 4, 5, 5-tetramethyl-1, 3, 2-dioxaborolan) carbazole



Under the protection of nitrogen, 3-bromocarbazole (60.95 mmol, 15 g), pinacol biborate (182.84 mmol, 43.68 g, 3 eq), potassium acetate (365.68 mmol, 35.89 g, 6 eq), palladium bistriphenylphosphine dichloride (6.095 mmol, 4.278 g, 0.1 eq) were dissolved in 500 mL of 1,4-dioxane. And the reaction was refluxed at 90℃ for 8 hours. After cooling to room temperature, extracted with dichloromethane and water,

the filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (2:1, v/v) as the eluent to give pure 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan) carbazole (15.724 g, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 8.19 (s, 1H), 8.11 (d, J = 7.8 Hz, 1H), 7.88 (dd, J = 8.1, 1.1 Hz, 1H), 7.44–7.38 (m, 3H), 7.26–7.22 (m, 1H), 1.40 (s, 12H).

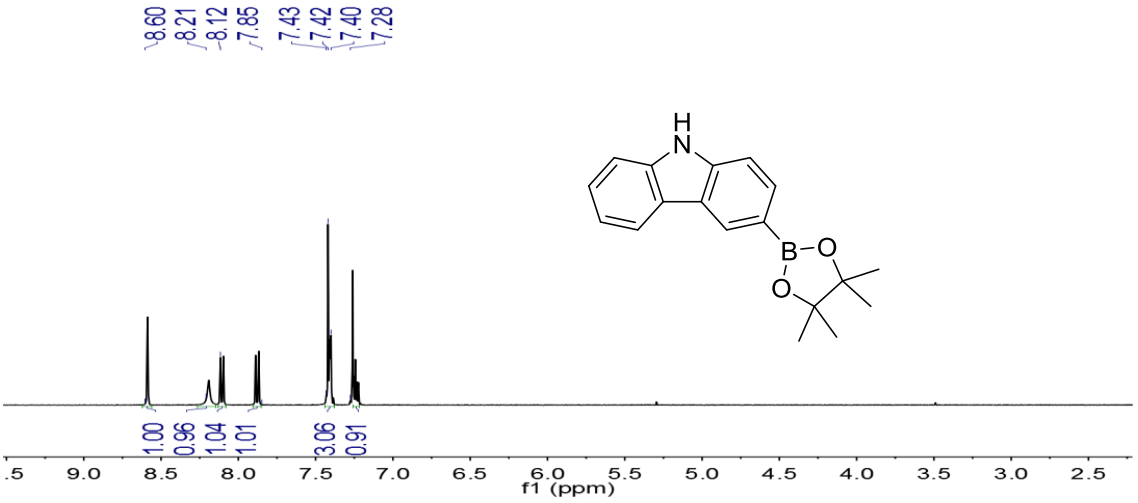
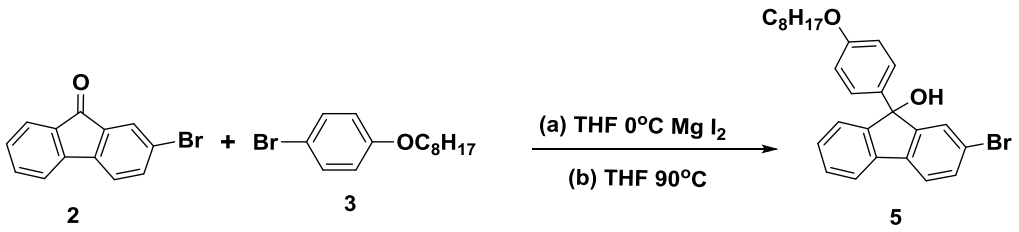


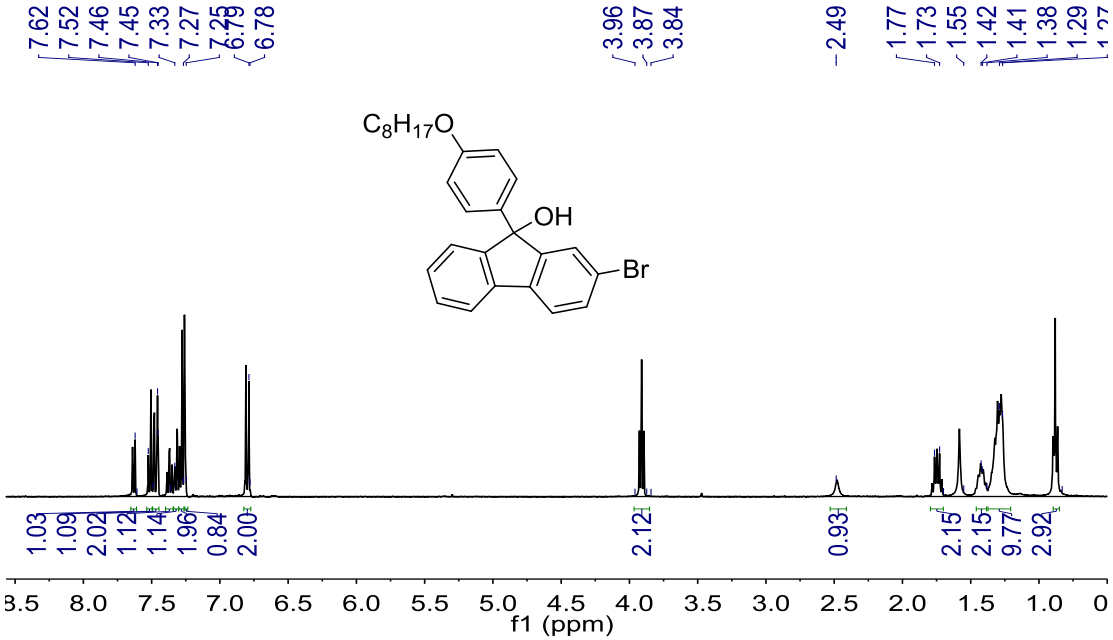
Figure S2. ^{1}H NMR spectrum of **4** recorded in $CDCl_3$

2.3 Compound **5**: 2-bromo-9-(4-octyl oxy phenyl) -9-fluorene -9-ol



Magnesium turning (1.6 mmol, 1.6 g), one piece of I_2, 20 mL of tetrahydrofuran and p-bromo -n- octyloxybenzene were added into a dry Schlenk tube. Then 5.00 mL of dry THF was added to disperse the powder under a nitrogen atmosphere. Then it was initiated by a heating gun, the solution changed from turbid to clear, and the reaction was completed. Then the mixture was antiferred to an oil bath at 55℃ for 3 hours until most magnesium fragments disappeared. Next, the above reaction solution

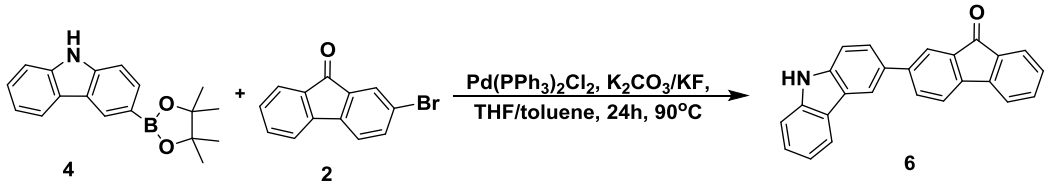
was antiferred to a reaction flask with 2-bromofluorenone (30 mmol, 7.76 g) and tetrahydrofuran (400 mL) and refluxed for 24 h. After the reaction was cooled to room temperature, the filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (1:1, v/v) as the eluent to give pure 2-bromo-9 -(4-octyl oxy phenyl) -9-fluorene -9-ol (65% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.6 Hz, 1H), 7.54–7.50 (m, 1H), 7.49–7.45 (m, 2H), 7.37 (td, J = 7.3, 1.5 Hz, 1H), 7.32 (d, J = 6.1 Hz, 1H), 7.30–7.26 (m, 2H), 7.25 (d, J = 3.1 Hz, 1H), 6.82–6.77 (m, 2H), 3.91 (t, J = 6.6 Hz, 2H), 2.48 (s, 1H), 1.79–1.70 (m, 2H), 1.37–1.21 (m, 10H), 0.87 (d, J =



7.0 Hz, 3H).

Figure S3. ^{1}H NMR spectrum of **5** recorded in $CDCl_3$

2.4 Compound **6**: 2-(9H-carbazol-3-yl)-9H-fluoren-9-one



2-bromofluorenone (27.29 mmol, 7.07 g), 3-carbazolylboronic acid pinacol

ester (40.93 mmol, 12 g, 1.5 eq), tetrabistriphenylphosphorpalladium (0.82 mmol, 0.95 g, 0.03 eq) were dissolved in 50 mL of Tol/THF (1:1, v/v) under a nitrogen atmosphere. Then 20 mL of dry K_2CO_3/KF was poured into the reaction and refluxed at 90 ℃ for 24 h. After the reaction was completed, it was quenched with water. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (3:1-2:1, v/v) as the eluent to give pure 2-(9H-carbazol-3-yl)-9H-fluoren-9-one (4.71 g, 50 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.16 (d, J = 8.0 Hz, 2H), 8.06 (s, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 7.8 Hz, 2H), 7.63 (d, J = 7.4 Hz, 1H), 7.58 (d, J = 7.2 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.49 (s, 2H), 7.32 (dd, J = 14.0, 6.4 Hz, 2H).

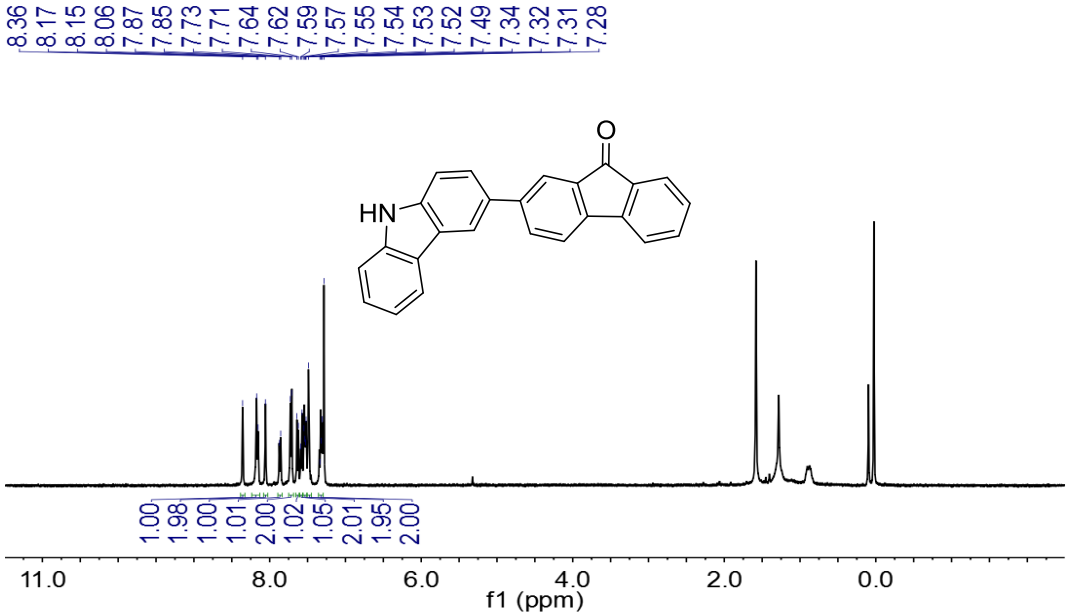
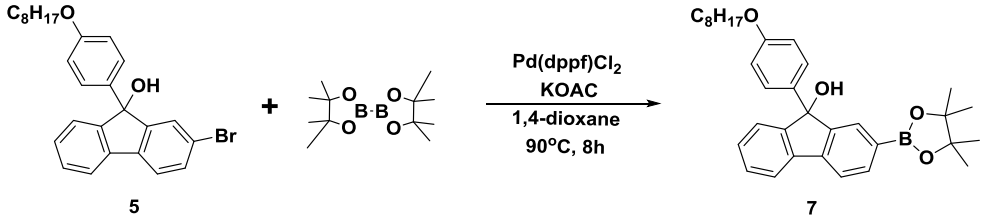


Figure S4. ^{1}H NMR spectrum of **6** recorded in $CDCl_3$

2.5Compound **7**: 9-(4-(octyloxy)phenyl)-2-(4,4,5,5,-teramethyl-1,3,2-dioxaborolan-2-yl)-9H-fluoren-9-ol



Under a nitrogen atmosphere, 2-bromo-9-(4-octyloxy)phenyl-9-fluorenol (17.18 mmol, 8 g), pinacol biborate (51.57 mmol, 13.09 g, 3 eq), potassium acetate (103.08 mmol, 10.17 g, 6 eq), bistriphenylphosphine palladium dichloride (1.718 mmol, 1.2 g, 0.1 eq) were dissolved in 300 mL of 1,4-dioxane. After that, the mixture was stirred at reflux overnight at 90 ℃. After cooling to room temperature, undissolved solid was filtered. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane-ethyl acetate (10:2:1, v/v) as the eluent to give pure 9-(4-(octyloxy)phenyl)-2-(4,4,5,5,-teramethyl-1,3,2-dioxaborolan-2-yl)-9H-fluoren-9-ol (6.34 g: 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, J = 7.5, 1.0 Hz, 1H), 7.78 (s, 1H), 7.67 (dd, J = 11.2, 4.1 Hz, 2H), 7.36 (td, J = 7.4, 1.3 Hz, 1 H), 7.34 – 7.30 (m, 2H), 7.30 – 7.26 (m, 2H), 7.25 (d, J = 1.0 Hz, 1H), 6.83–6.75 (m, 2H), 3.91 (t, J = 6.6 Hz, 2H), 2.49 (s, 1H), 1.79 ‑ 1.70 (m, 2H), 1.42 (dd, J = 15.1, 6.9 Hz, 2H), 1.35 ‑ 1.25 (m, 20H), 0.88 (t, J = 6.9 Hz, 3H).

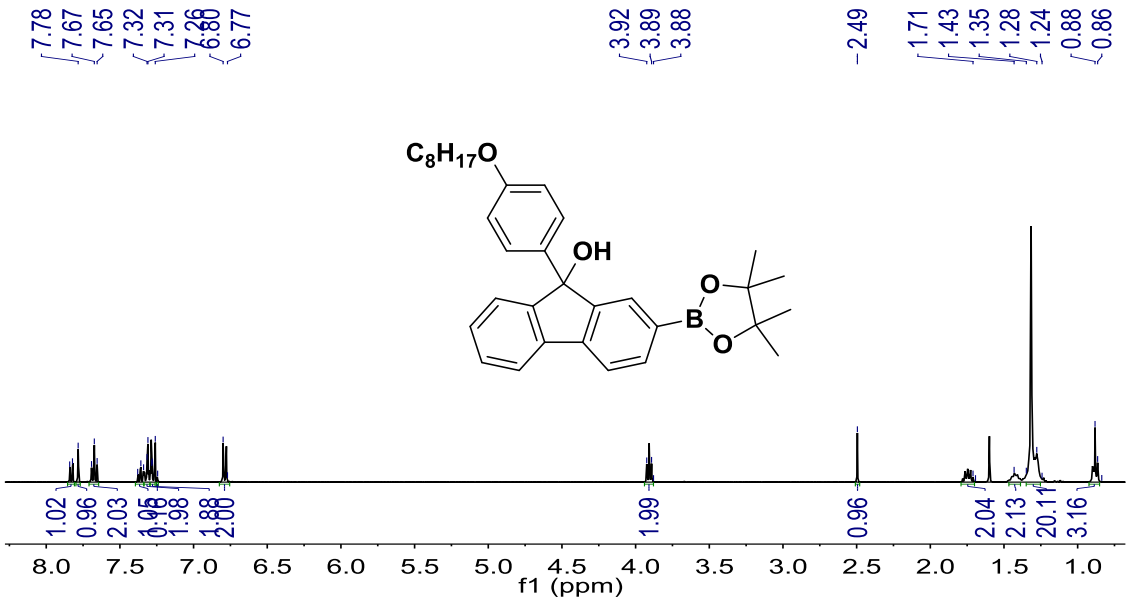
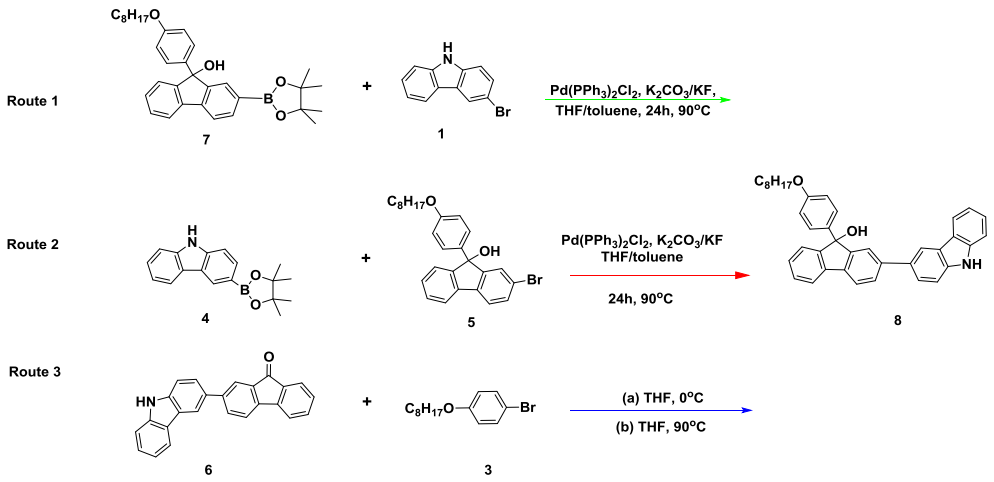


Figure S5. ^{1}H NMR spectrum of **7** recorded in $CDCl_3$

2.6 Compound **8**: 2-(9H-carbazol-3-yl)-9-(4-octyloxy)phenyl) -9H-fluoren-9-ol



Route 1: 9-(4-n-octyloxyphenyl)-9-hydroxy-2-fluorene boronic acid pinacol ester (7.80 mmol, 4g), 3-bromocarbazole (11.7 mmol, 2.88 g, 1.5 eq), tetrabistriphenylpalladium (0.23 mmol, 0.27 g, 0.03 eq) were added to the three-necked flask under a nitrogen atmosphere reaction. Then 10.00 mL of dry Tol/THF (1:1, v/v) was added to disperse the powder. Under the protection of argon, the suspension was stirred at 90°C for 20 min, 30 mL of aqueous solution was poured into the reaction device, and refluxed at 90 ℃ for 24 h. After cooling to room temperature, undissolved solid was filtered. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (4:1-1:1, v/v) as the eluent to give pure 2-(9H-carbazol-3-yl)-9-(4-octyloxy)phenyl) -9H-fluoren-9-ol (2.37 g, 53%).

Route 2: 2-bromo-9-(4-n-octyloxyphenyl)-9-fluoren-9-ol (8.59 mmol, 4 g), 3-carbazole boric acid pinacol ester (12.89 mmol, 3.78 g, 1.5 eq), tetrabistriphenylphosphorpalladium (0.26 mmol, 0.30 g, 0.03 eq) was dissolved in 50 mL of Tol/THF (1:1, v/v) at 90 ℃ for 20 min under a nitrogen atmosphere. Then 30 mL of K_2CO_3 (2 M) / KF was added to disperse the powder and degassed in liquid nitrogen three times, and refluxed at 90 ℃ for 24 h. After cooling to room temperature, undissolved solid was filtered. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (4:1-1:1, v/v) as the eluent to give pure 2-(9H-carbazol-3-yl)-9-(4-octyloxy)phenyl) -9H-fluoren-9-ol (2.6 g, 55%).

Route 3: Magnesium turning (25 mmol, 0.61 g), a grain of iodine, 10 mL of tetrahydrofuran, a small amount of p-bromo-n-octyloxybenzene (24 mmol, 6.85 g, 2 eq) were added into a dry Schlenk tube. Then 30.00 mL of dry THF was added to disperse the powder under a nitrogen atmosphere. Then it was initiated by a heating gun, the solution changed from turbid to clear, and the reaction was completed. Then the mixture was antiferred to an oil bath at 55℃ for 3 hours until most magnesium fragments disappeared. Next, the above reaction solution was antiferred to a reaction flask with 2-(9H- carbazole -3- yl)-fluorenone (11.58 mmol, 4 g) and tetrahydrofuran (400 mL) at 90ºC for 24 h. After the reaction was cooled to room temperature, the filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography using petroleum ether-dichloromethane (4:1, v/v) as the eluent to give pure 2-(9H-carbazol-3-yl)-9-(4-octyloxy)phenyl) -9H-fluoren-9-ol (3.51 g, 49%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 1.4 Hz, 1H), 8.10 (t, J = 7.2 Hz, 1H), 8.07 (s, 1H), 7.72 (d, J = 14.8, 9.3, 5.8 Hz, 4H), 7.62 (dd, J = 8.4, 1.8 Hz, 1H), 7.45 – 7.40 (m, 3H), 7.38 (dd, J = 8.0, 2.5 Hz, 4H), 7.28 (dd, J = 5.7, 1.7 Hz, 1H), 7.26 – 7.23 (m, 1H), 6.82 (d, J = 8.9 Hz, 2H), 3.90 (t, J = 6.6 Hz, 2H), 2.59 (s, 1H), 1.78 – 1.70 (m, 2H), 1.28 (s, 10H), 0.88 (d, J = 4.7 Hz, 3H).

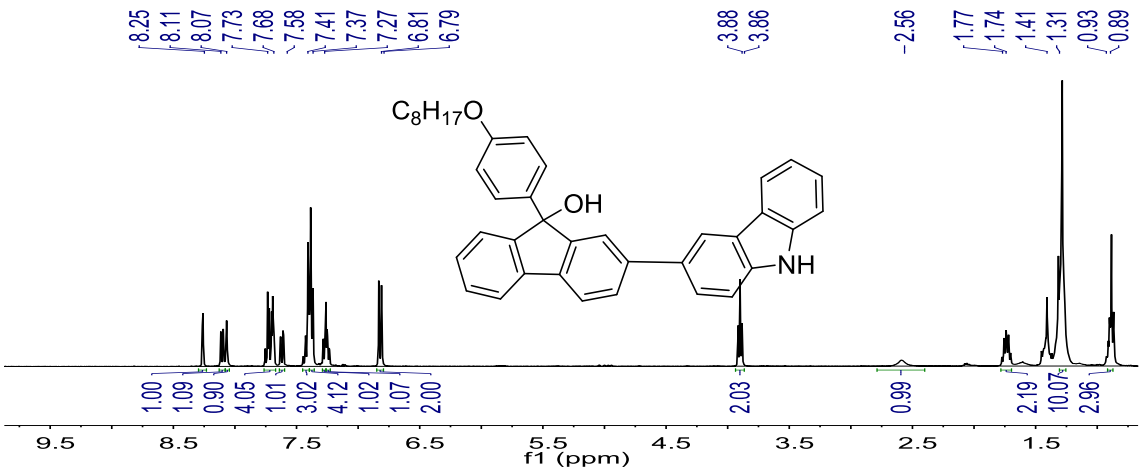
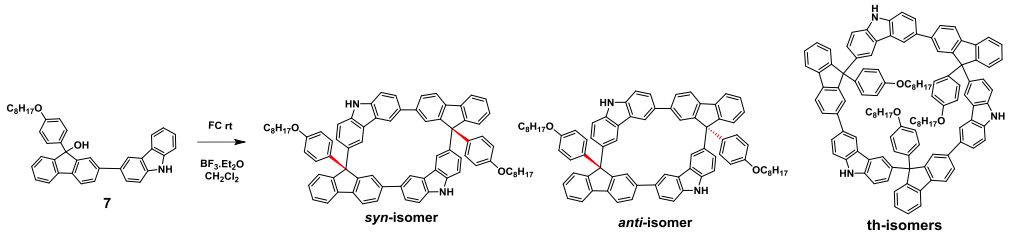


Figure S6. ^{1}H NMR spectrum of **8** recorded in $CDCl_3$

2.7 Syntheses of ***syn*-isomer**, ***anti*- isomer** and **th-isomer**



The synthon **7** (0.91 mmol, 0.5 g) was dissolved in 500 mL of methylene chloridconstant at pressure titration funnel and dropped into the reaction bottle with 1 mL boron trifluoride ether. Water was used to quench the reaction after it was completed. The organic layer was then separated from the aqueous layer, and dried with anhydrous Na_2SO_4. The filtrate was concentrated under reduced pressure to obtain the crude product, which was purified by column chromatography to obtain pure ***syn*-isomer** (0.12 g, 25%) MADLI-TOF-MS (m/z): cacld. For $C_{78}H_{70}N_2O_2$: 1066.543 [M+]; Found: 1066.881. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, J = 1.3 Hz, 2H), 8.59 (s, 2H), 8.24 (s, 2H), 7.96 (s, 2H), 7.85 (d, J = 7.4 Hz, 2H), 7.82 (d, J = 7.9 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 7.6 Hz, 2H), 7.55 (d, J = 7.4 Hz, 2H), 7.45 (t, J = 7.0 Hz, 2H), 7.41 – 7.35 (m, 2H), 7.32 – 7.28 (m, 2H), 7.28 – 7.25 (m, 2H), 7.18 (d, J = 8.5 Hz, 2H), 7.14 (d, J = 8.9 Hz, 4H), 6.76 (d, J = 9.0 Hz, 4H), 3.89 (t, J = 6.6 Hz, 4H), 1.78–1.70 (m, 4H), 1.31 (d, J = 7.6 Hz, 20H), 0.89 (t, J = 6.9 Hz, 6H).

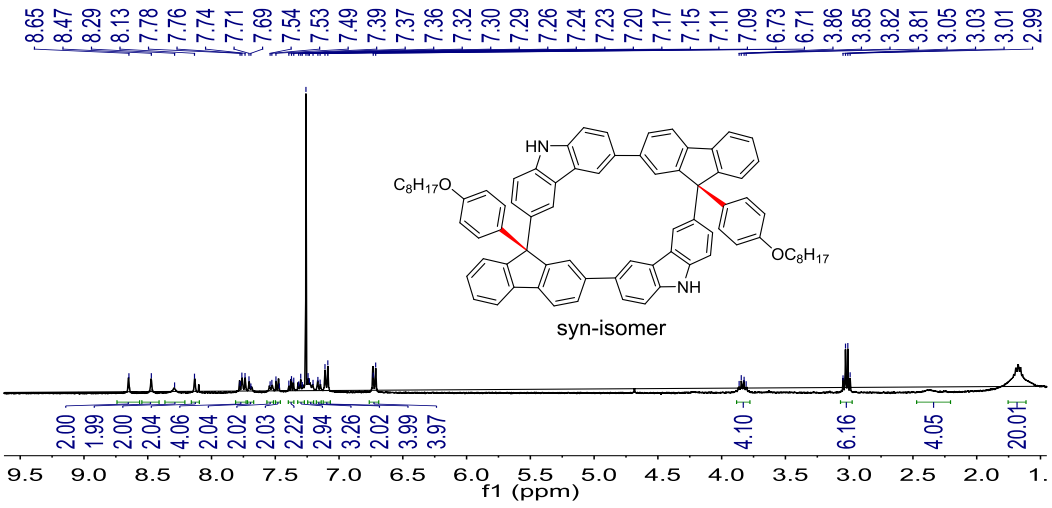


Figure S7. ^{1}H NMR spectrum of ***syn*-isomer** recorded in $CDCl_3$

Then the second separation was carried out, using petroleum ether-dichloromethane (4:1-3:1, v/v) as the eluent to obtain ***anti*-isomer** (0.04 g, 9%) MADLI-TOF-MS (m/z): cacld. For $C_{78}H_{70}N_2O_2$: 1066.543 [M+]; Found: 1066.887. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (s, 2H), 8.34 (s, 2H), 8.29 (s, 2H), 8.04 (s, 2H), 7.91 (d, J = 7.7 Hz, 4H), 7.64 (d, J = 7.0 Hz, 6H), 7.57 (d, J = 8.0 Hz, 4H), 7.48 (t, J = 7.4 Hz, 2H), 7.45 – 7.37 (m, 4H), 6.77 (d, J = 8.7 Hz, 4H), 6.60 (d, J = 8.8 Hz, 4H), 3.79 (t, J = 6.6 Hz, 4H), 1.66 (d, J = 6.6 Hz, 4H), 1.29 (d, J = 10.4 Hz, 20H), 0.85 (d, J = 6.7 Hz, 6H).

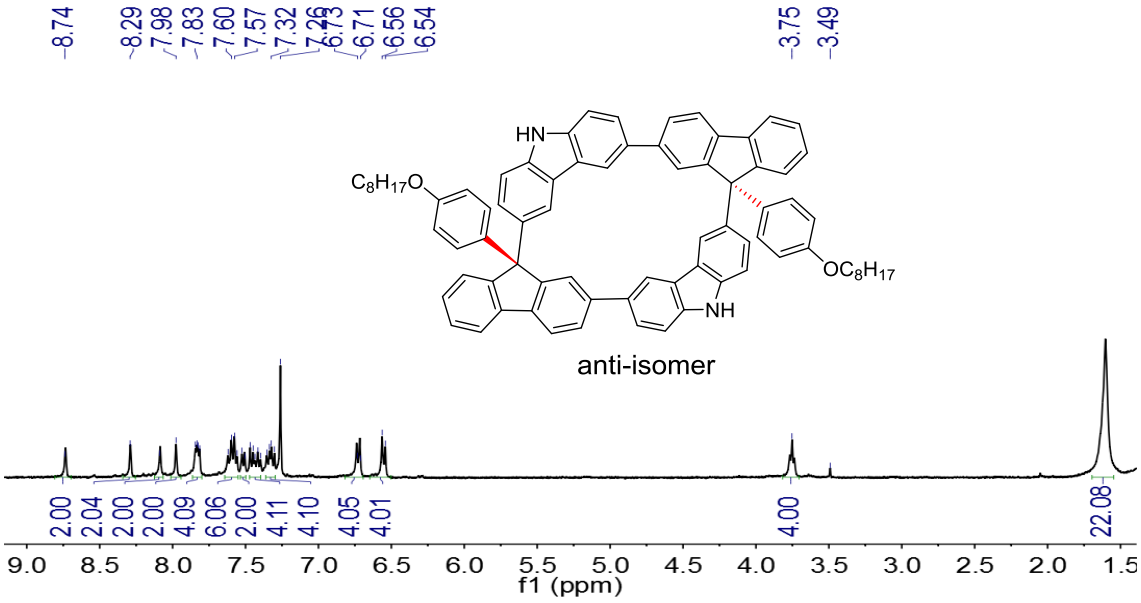


Figure S8. ^{1}H NMR spectrum of ***anti*-isomer** recorded in $CDCl_3$

Petroleum ether-dichloromethane (3:1-2:1, v/v) was used as the eluent to obtain **th-isomer** (0.07 g, 6%) MADLI-TOF-MS (m/z): cacld. For $C_{117}H_{105}N_3O_3$: 1601.302[M+]; Found: 1061. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (dd, J = 25.7, 14.7 Hz, 2H), 8.39 – 8.25 (m, 2H), 8.18 (s, 1H), 8.07 – 8.00 (m, 3H), 7.97 (d, J = 6.0 Hz, 1H), 7.92 (d, J = 5.6 Hz, 1H), 7.90 (s, 1H), 7.84 (dd, J = 8.2, 3.3 Hz, 3H), 7.81 – 7.76 (m, 2H), 7.72 (d, J = 7.5 Hz, 2H), 7.68 – 7.61 (m, 2H), 7.60 – 7.55 (m, 2H), 7.52 (dd, J = 10.7, 7.0 Hz, 3H), 7.49 (s, 1H), 7.47 – 7.44 (m, 2H), 7.43 – 7.40 (m, 3H), 7.40 – 7.36 (m, 2H), 7.35 (s, 1H), 7.33 (s, 1H), 7.30 (d, J = 3.4 Hz, 1H), 7.22 (d, J = 8.7 Hz, 3H), 7.19 – 7.15 (m, 1H), 7.08 – 7.01 (m, 1H), 6.98 – 6.89 (m, 1H), 6.86 (d, J = 10.0

Hz, 1H), 6.79 (dd, J = 14.8, 8.9 Hz, 2H), 6.74 (dd, J = 8.8, 3.0 Hz, 2H), 6.66 (d, J = 8.9 Hz, 1H), 6.56 (dd, J = 11.4, 5.1 Hz, 3H), 6.45 (d, J = 9.0 Hz, 1H), 3.94 (dd, J = 12.2, 6.1 Hz, 2H), 3.75 (t, J = 6.3 Hz, 3H), 3.61 (t, J = 6.6 Hz, 1H), 1.82 – 1.63 (m, 6H), 1.35 (dd, J = 71.0, 21.8 Hz, 39H).

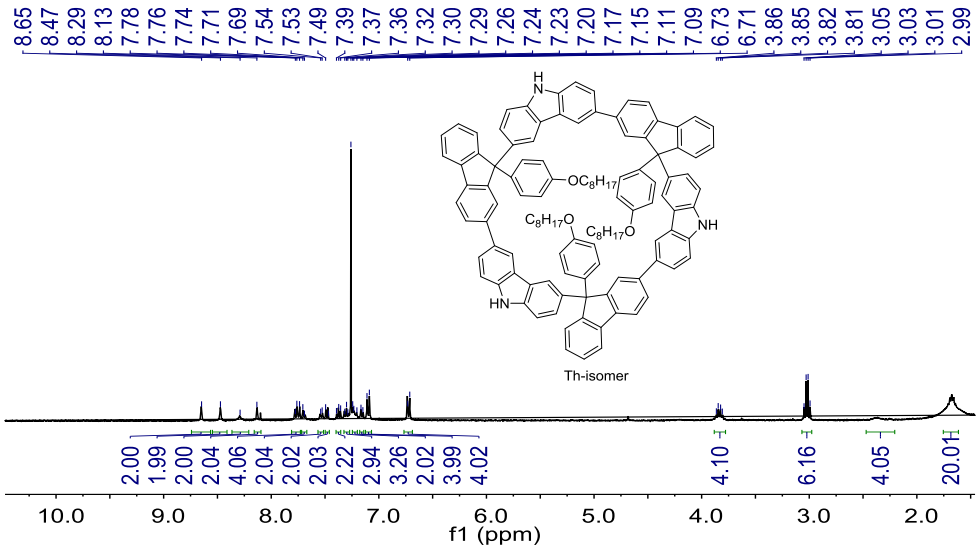
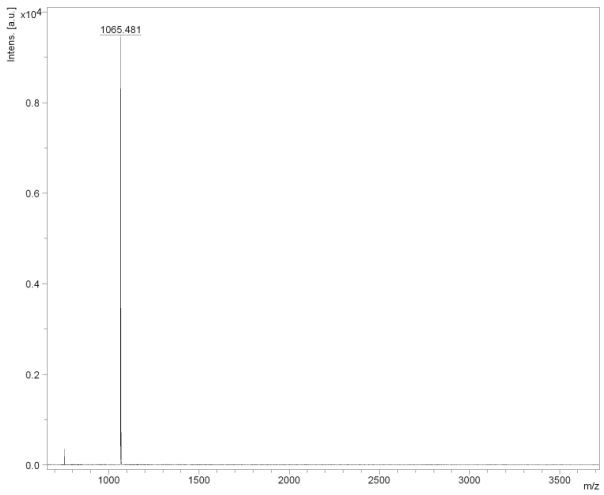
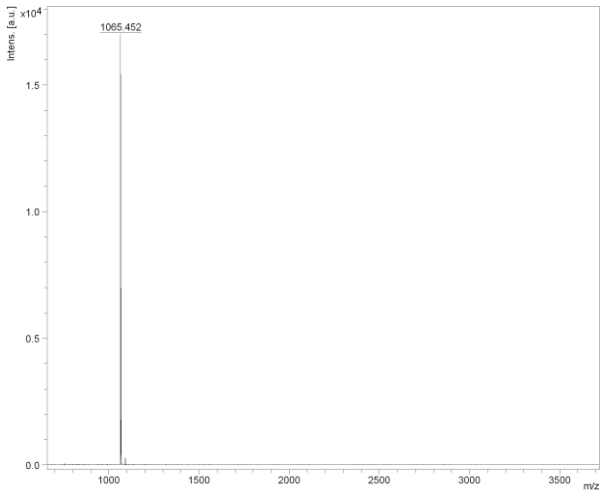


Figure S9. ^{1}H NMR spectrum of **th-isomer** recorded in $CDCl_3$

3. MALDI-TOF-MS of ***syn/anti*** **isomers**



(a)



(b)

Figure S10. MALDI-TOF mass spectrum of ***syn/anti* isomers**: (a) *syn*-isomer (b) *anti*-isomer

4. ^{1}H NMR of the ***syn/anti* isomers**

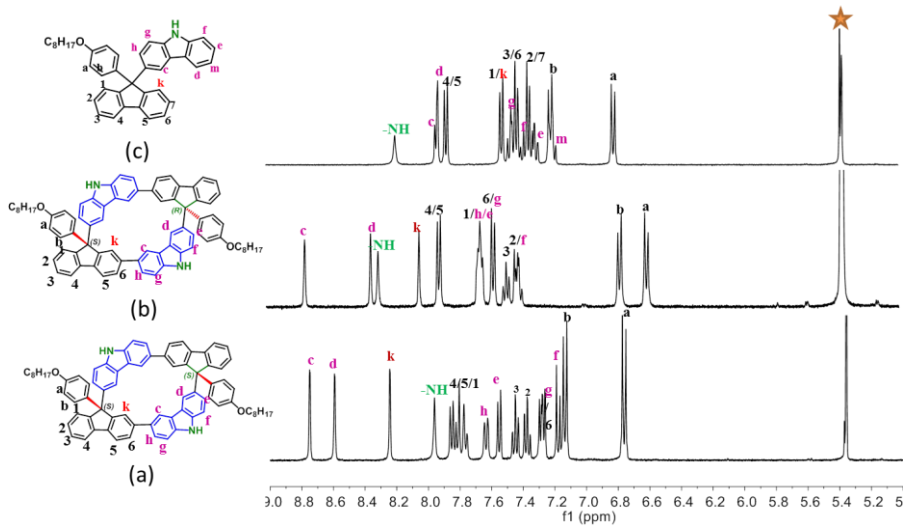


Figure S11. ^{1}H NMR spectrum of ***syn*/*anti* isomer** recorded in CD_2Cl_2: (a) *syn*-isomer (b) *anti*-isomer

In order to better perform NMR analysis, we have synthesized the L-shaped molecule (**c**) and compared it with the two isomers in NMR spectra, as shown in Figure S11. In the Friedel-Crafts reaction, the **m** position in compound **c** is connected to the **3** position of another **c** molecule, causing the proton **d** to change from the original double peak to single peak, and it is in the de-shielding zone, so the electron cloud density decreases and shifts to low field. Moreover, due to the strong shielding effect of the isomers, the chemical shift of proton **d** is in a lower field. Proton **k** is

changed from the original double peak to single peak due to the ring reaction of the **7**-position hydrogen atom. Due to the influence of carbazole, the unshielded zone of proton **k** is stronger than before, and its chemical shift shifts to a low field. The single crystal X-ray diffraction data confirms the results.

5. Optimized geometries of the two isomers of the 1:1 complex in gas phase by Gaussian computer program

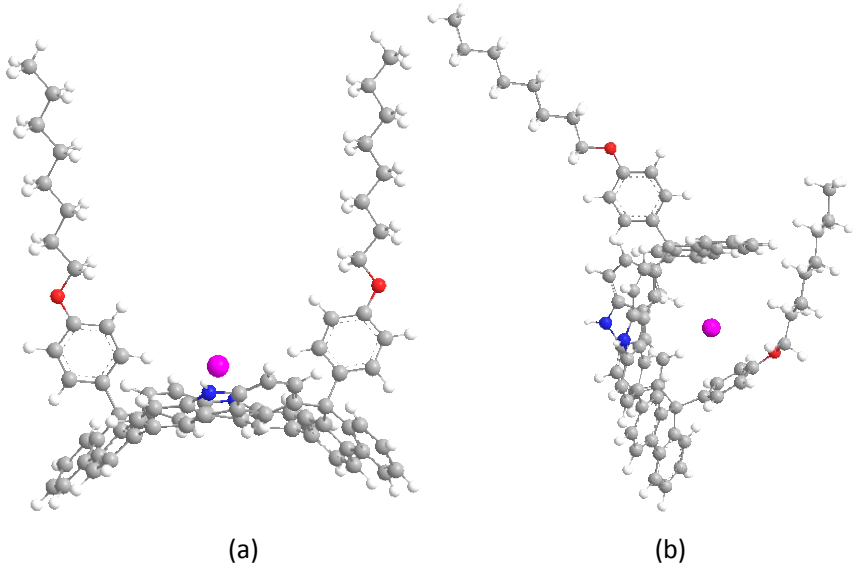


Figure S12. Energy-minimized structures of the two isomers of the 1:1 complex: (a) ***syn*-isomer** (b) ***anti*-isomer** (Nitrogen atoms are blue, oxygen atoms are red, hydrogen atoms are white, and iodine atoms are purple)

Computations were carried out by DFT methods in Gaussian 16 with a dispersion correction DFT-D3 (BJ).[1] B3LYP method with 6- 31G* basis set were employed to investigate the structure optimization. The Stuttgart–Dresden double-zeta valence basis set (SDD) with an effective core potential for 46 inner electrons was employed for iodine. Since the program uses a larger system with more basis functions, and an alternative basis function for a smaller system, there is basis set overlap error in the entire optimization calculation. We used the correction method proposed by Boys and Bernardi to perform the basis set superposition error (BSSE).[2] The optimized energies obtained for ***syn*-isomer** I^- complex and ***anti*-isomer** I^- complex are shown in Table S1.

Table S1 Optimized energies obtained for the two isomers of the 1:1 complex in gas phase at 298 K

***syn*-isomer I^- complex**	Value / Hartree	***anti*-isomer I^- complex**	Value/Hartree
$E_{\textbf{\textit{syn}-isomer } I^-}$	-3286.03030	$E_{\textbf{\textit{anti}-isomer } I^-}$	-3286.04059
$E_{\textbf{\textit{syn}-isomer}}$	-3274.90734	$E_{\textbf{\textit{anti}-isomer}}$	-3274.90543
E_{I^-}	-10.93511	E_{I^-}	-10.93511
$E_{\textbf{\textit{syn}-isomer}(BSSE)}$	-3274.83761	$E_{\textbf{\textit{anti}-isomer}(BSSE)}$	-3274.83529
$E_{I^-(BSSE)}$	-10.93703	$E_{I^-(BSSE)}$	-10.93511
$\triangle E_{cor(BSSE)}$	0.00412	$\triangle E_{cor(BSSE)}$	0.00616
$\triangle E$	-0.18785	$\triangle E$	-0.20005
$\triangle E_{BSSE}$	-0.18373	$\triangle E_{BSSE}$	-0.19389

$\triangle E = E_{\textbf{isomer } I^-} - (E_{\textbf{isomer}} + E_{I^-})$

$\triangle EBSSE = \triangle E + \triangle E_{cor(BSSE)}$

$\triangle E_{cor(BSSE)}$ is calculated by Gaussian software.

6. UV-visible absorption of ***syn/anti* isomers** in CH_2Cl_2 solution

Stock solutions of all the compounds studied were made up in CH_2Cl_2. ACS grade solvents were purchased and used without purification. The stock solutions were appropriately diluted with solvents to obtain concentrations suitable for study.

6. 1 UV-vis spectra of ***syn*-isomer** recorded in CH_2Cl_2 after adding excess quantities of the indicated anions as their TBA+ (tetrabutylammonium) salts (TBAF, TBACl and TBABr)

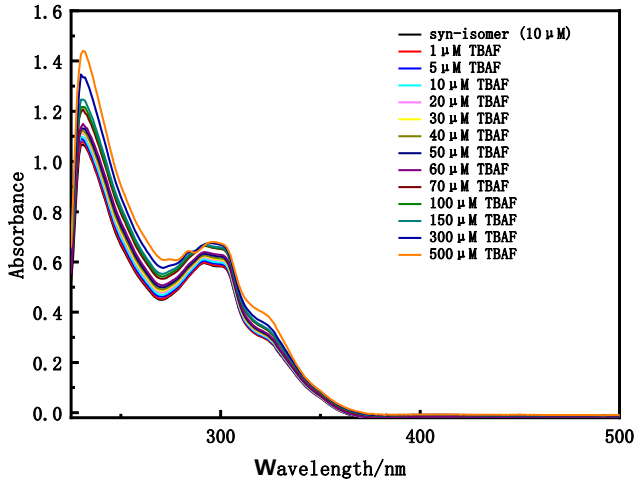


Figure S13. UV-vis spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBAF (tetrabutylammonium fluoride, 0~50 eq)

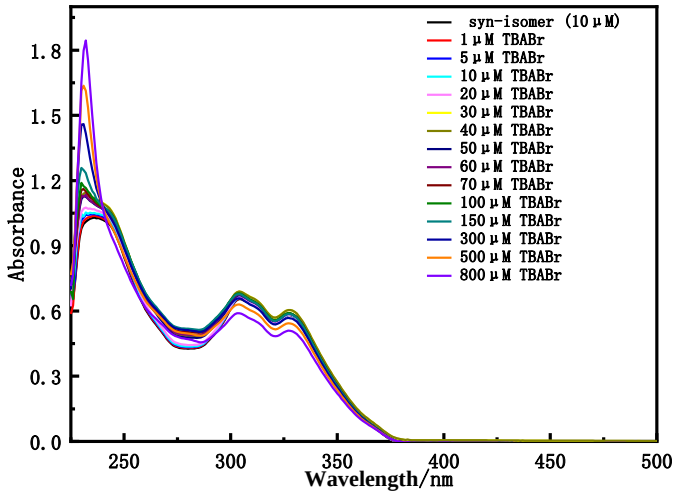


Figure S14. UV-vis spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBACl (tetrabutylammonium chloride, 0~50 eq)

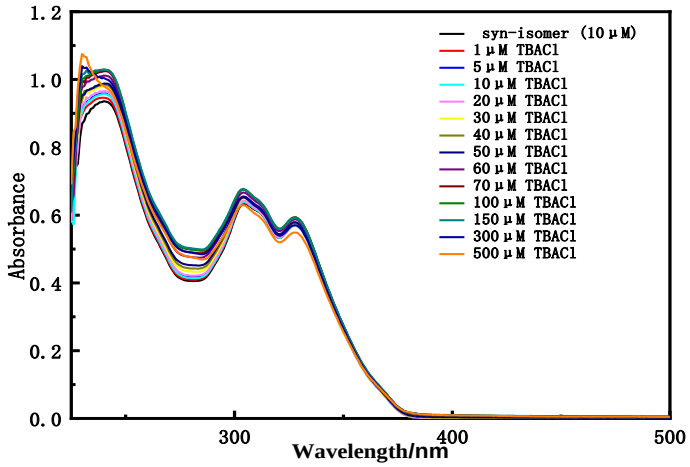


Figure S15. UV-vis spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBABr (tetrabutylammonium bromide, 0~80 eq)

6.2 UV-vis spectra of ***anti*-isomer** recorded in CH_2Cl_2 after adding excess quantities of the indicated anions as their TBA+ (tetrabutylammonium) salts (TBAF, TBACl and TBABr)

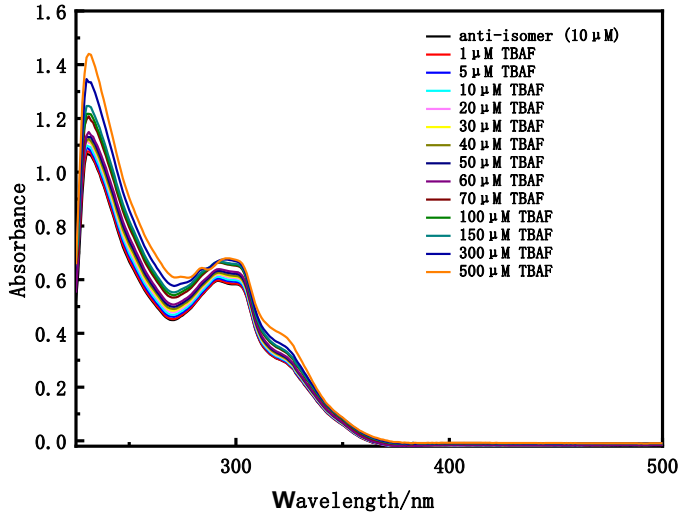


Figure S16. UV-vis spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBAF (tetrabutylammonium fluoride, 0~50 eq)

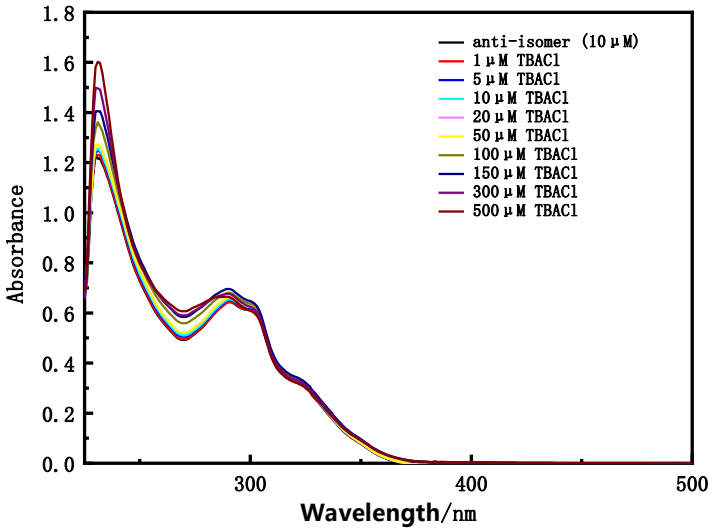


Figure S17. UV-vis spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBACl (tetrabutylammonium chloride, 0~50 eq)

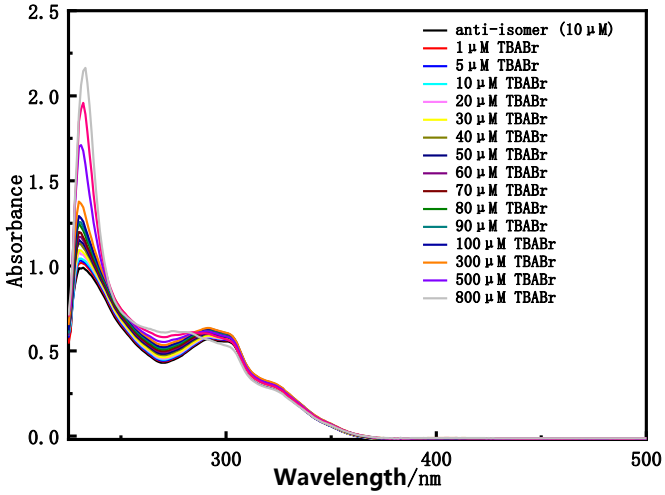


Figure S18. UV-vis spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBABr (tetrabutylammonium bromide, 0~80 eq)

7. Binding constants determined by UV-vis itrations

Upon addition of incremental amounts of anions to a CH_2Cl_2 solution of ***syn/anti* isomers**, changes in the absorbance features of ***syn/anti* isomers** (10 μM was used, unless otherwise stated) were seen.

7.1 Binding constants[3] determined by UV-vis itrations of ***syn*-isomer**

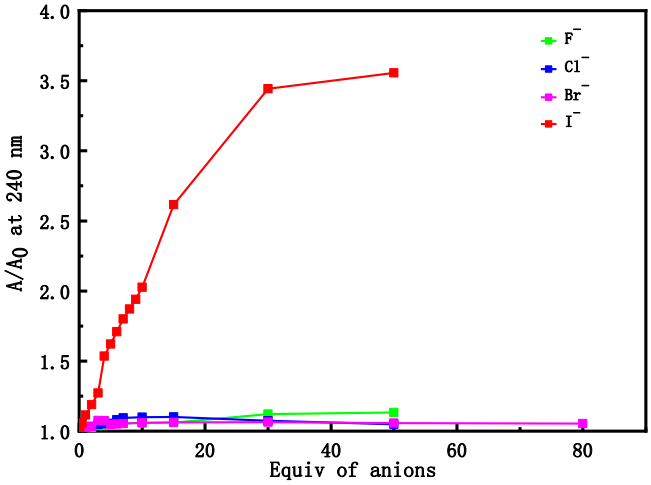


Figure S19. The corresponding binding isotherm for TBA+ (tetrabutylammonium) salts (TBAF, TBACl, TBABr and TBAI).

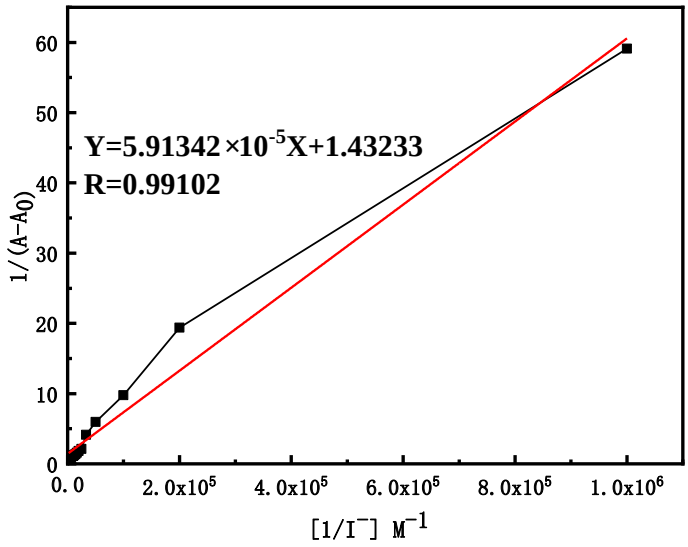


Figure S20. The Benesi-Hilderbrand diagram of ***syn*-isomer** with TBAI (tetrabutylammonium iodide)

Table S2 Calculation of the association constant of ***syn*-isomer** with TBAI (tetrabutylammonium iodide)

Y=A+BX		
coefficient	value	error
A	1.43233	0.58714
B	$5.91342E^{-5}$	$2.21333E^{-6}$
$KS = A/B = 2.422\times10^4$		
$\Delta K_S = \lvert\Delta A/A-\Delta B/B\rvert\times K_S = 0.902\times10^4$		
$K= K_S+\Delta K_S = (2.422\pm0.902)\times10^4$		

7.2 Binding constants determined by UV-vis itrations of ***anti*-isomer**

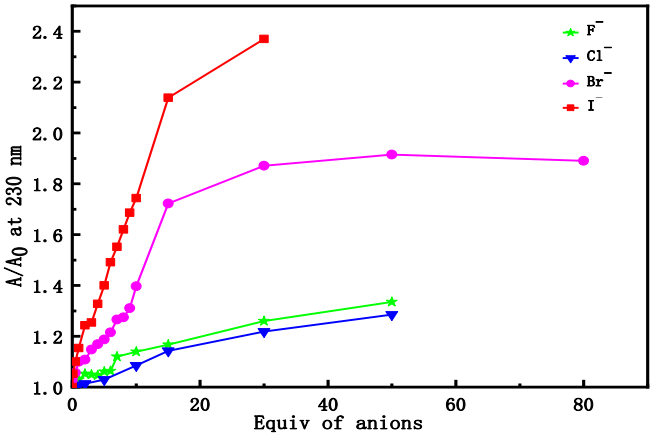


Figure S21. The corresponding binding isotherm for TBA+ (tetrabutylammonium) salts (TBAF, TBACl, TBABr and TBAI).

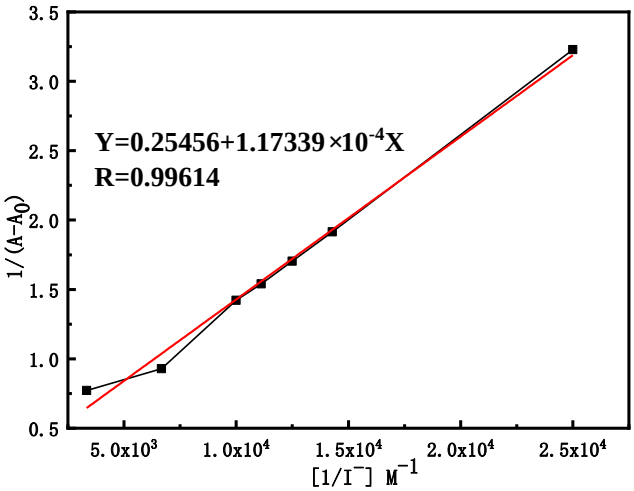


Figure S22. The Benesi-Hilderbrand diagram of ***anti*-isomer** with TBAI (tetrabutylammonium iodide)

Table S3 Calculation of the association constant K of ***anti*-isomer** with TBAI (tetrabutylammonium iodide)

Y=A+BX		
coefficient	value	error

A	0.25456	0.06218
B	$1.173992E^{-4}$	$4.62657E^{-6}$
$KS = A/B = 2.168 \times 10^3$		
$\Delta K_S = \lvert \Delta A/A - \Delta B/B \rvert \times K_S = 0.445 \times 10^3$		
$K = K_S + \Delta K_S = (2.168 \pm 0.445) \times 10^3$		

8. Fluorescence emission spectra of ***syn/anti* isomers** in CH_2Cl_2 solution

Stock solutions of all the compounds studied were made up in CH_2Cl_2. ACS grade solvents were purchased and used without purification. The stock solutions were appropriately diluted with solvents to obtain concentrations suitable for study.

8.1 Fluorescence emission spectra of ***syn*-isomer** recorded in CH_2Cl_2 after adding excess quantities of the indicated anions as their TBA+ (tetrabutylammonium) salts (TBAF, TBACl and TBABr)

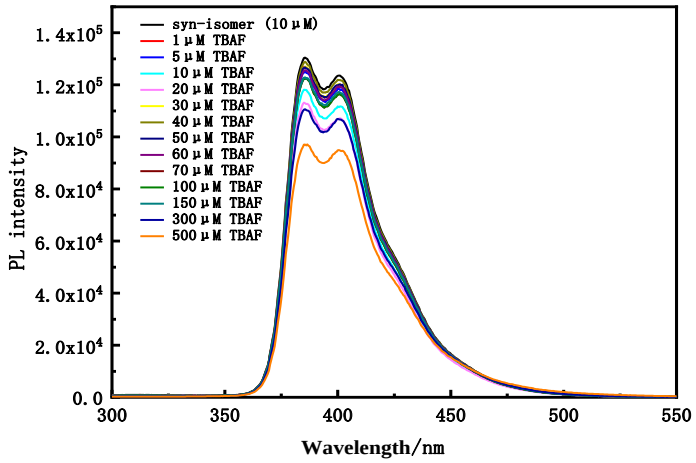


Figure S23. Fluorescence spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBAF (tetrabutylammonium fluoride, 0~50 eq)

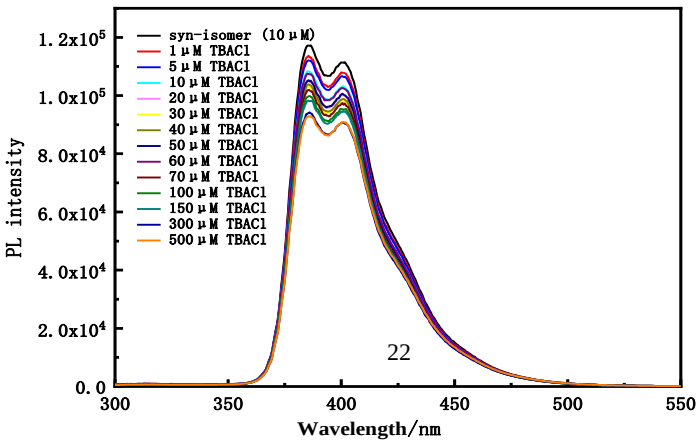


Figure S24. Fluorescence spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBACl (tetrabutylammonium chloride, 0~50 eq)

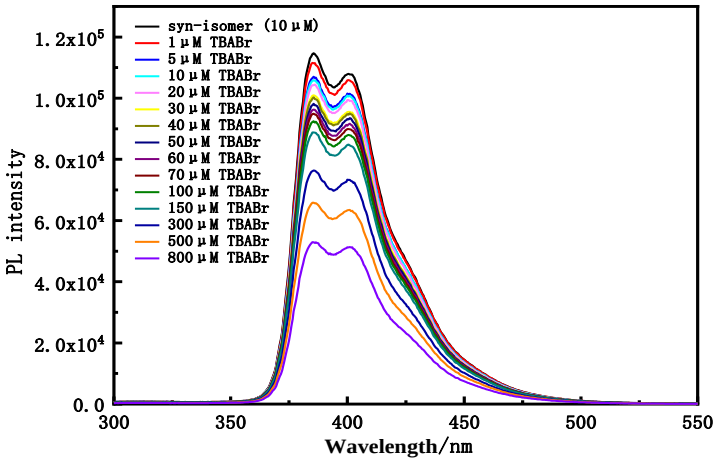


Figure S25. Fluorescence spectra of ***syn*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBABr (tetrabutylammonium bromide, 0~80 eq)

8.2 Fluorescence emission spectra of ***anti*-isomer** recorded in CH_2Cl_2 after adding excess quantities of the indicated anions as their TBA+ (tetrabutylammonium) salts (TBAF, TBACl and TBABr)

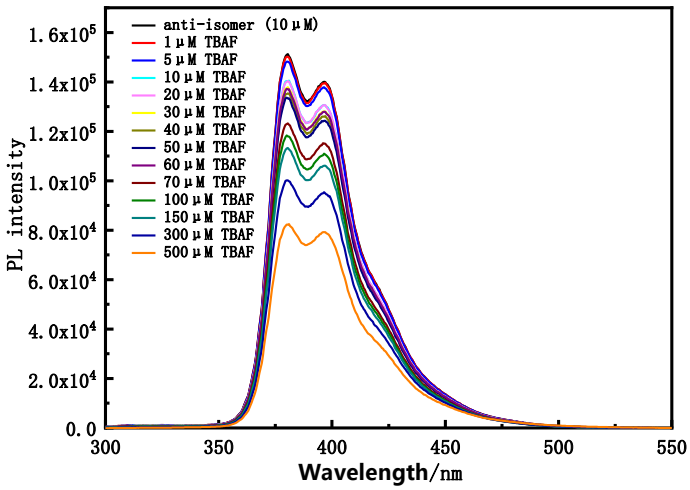


Figure S26. Fluorescence spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBAF (tetrabutylammonium fluoride, 0~50 eq)

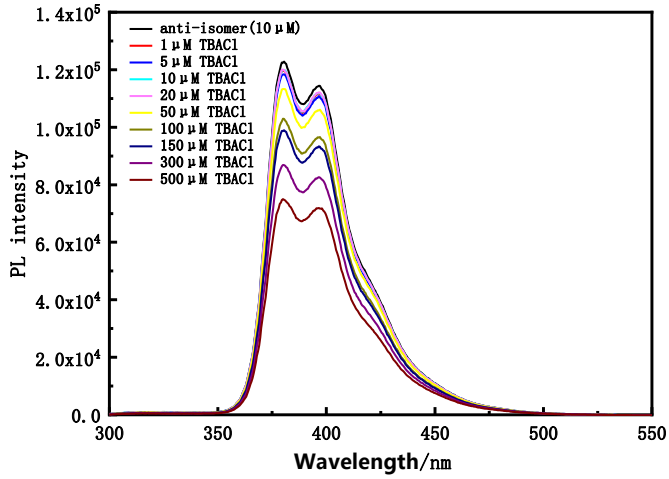


Figure S27. Fluorescence spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBACl (tetrabutylammonium chloride, 0~50 eq)

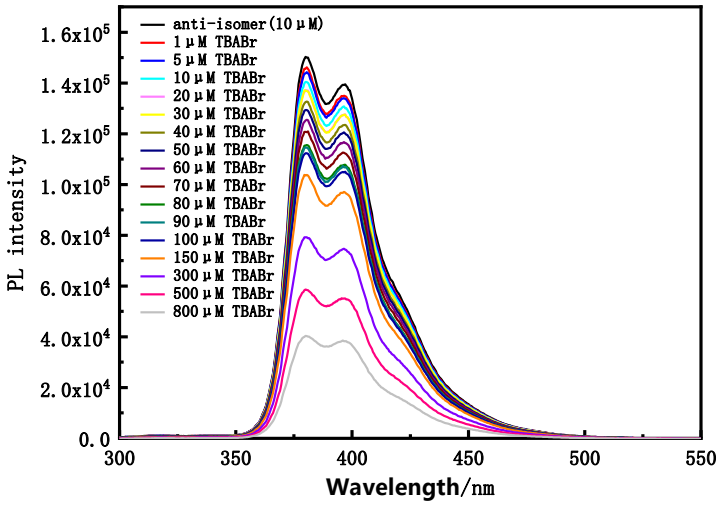


Figure S28. Fluorescence spectra of ***anti*-isomer** (10 μM) recorded in CH_2Cl_2 in the presence of increasing quantities of TBABr (tetrabutylammonium bromide, 0~80 eq)

9. Fluorescence spectral changes of ***syn/anti* isomers** in CH_2Cl_2

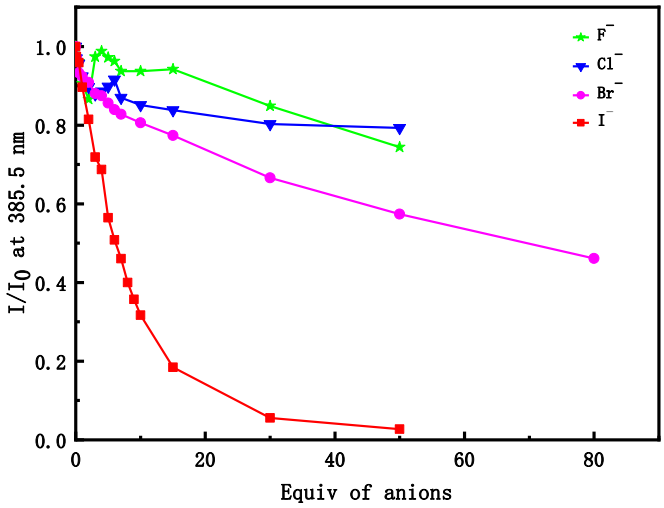


Figure S29. Fluorescence spectrum changes of ***syn*-isomer** in CH_2Cl_2 interacting with TBAX (TBAF, TBACl, TBABr and TBAI)

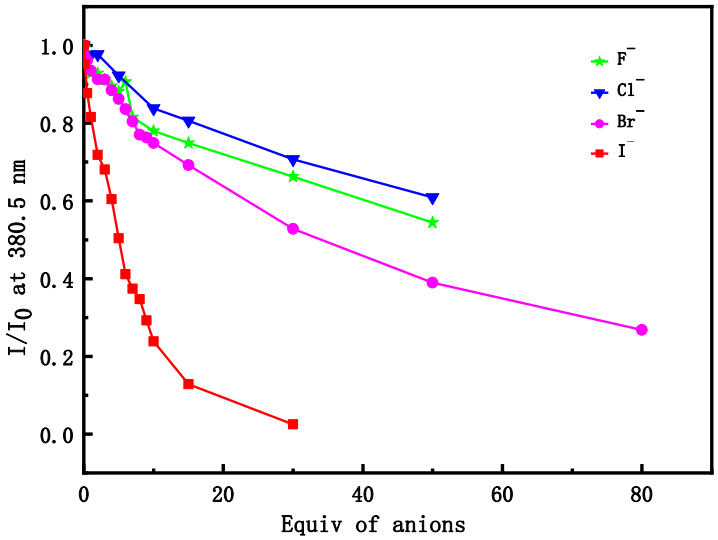
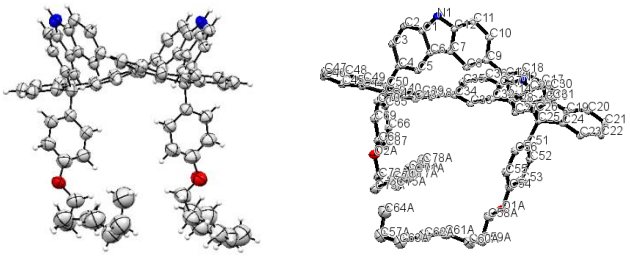


Figure S30. Fluorescence spectrum changes of ***anti*-isomer** in CH_2Cl_2 interacting with TBAX (TBAF, TBACl, TBABr and TBAI)

10. Single crystal X-ray diffraction data for ***syn*-isomer**



(a) (b)

Figure S31. Single crystal structure and ellipsometry of ***syn*-isomer**

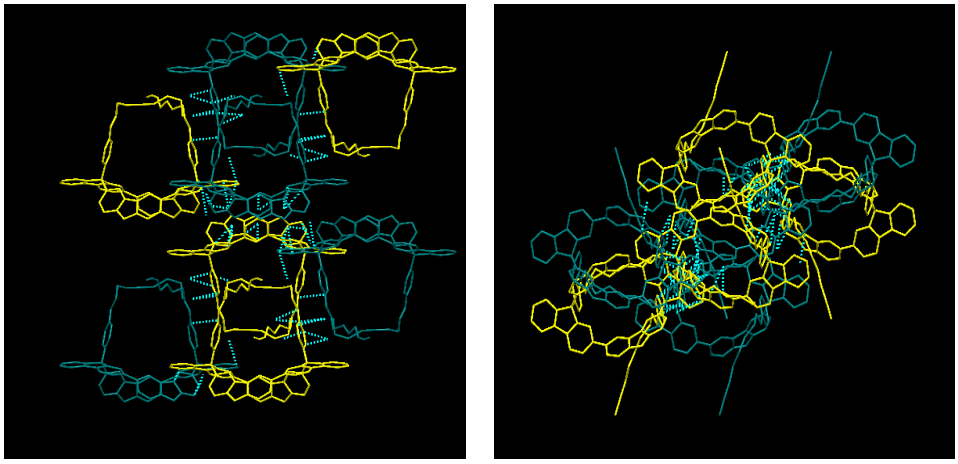


Figure S32. Interaction forces in ***syn*-isomer** single crystal

Table S4 Single crystal data of ***syn*-isomer**

Name	***syn*-isomer**
CCDC NO.	1911554
Formula sum	C78H70N2O2
Formula weight	1067.36g/mol
Crystal system	orthorhombic
Space-group	P b c a (61)
a [Å]	21.2514(3)
b [Å]	16.3136(3)
c [Å]	36.1817(6)
a/b	1.3027
b/c	0.4509
c/a	1.7026
Cell volume	12543.72(40) $Å^3$
z	8

Calc. density	1.13031g/cm^3
Rall	0.1597
Pearson code	oP1632
Formula type	NOP35Q39
Wyckoff sequence	c204

11. Cartesian coordinates of the optimized compounds

***Anti*-isomer：**

C	-1.25630700	0.94507700	3.02042100
C	-0.28528300	-0.05293700	3.46531700
C	-0.31294600	-0.02342000	4.88863000
N	-1.25528600	0.89880800	5.30127300
C	-1.85036600	1.47748400	4.19510800
C	-2.88438400	2.41090000	4.14139600
C	-3.29074800	2.84797200	2.89116400
C	-2.67128300	2.41159900	1.69885200
C	-1.66297400	1.44637800	1.77157500
C	0.54482700	-0.98801900	2.82745300
C	1.35039400	-1.85362600	3.58760000
C	1.34149300	-1.72641800	4.99858300
C	0.51503900	-0.83378300	5.66111300
C	4.84252800	-5.78920900	1.27824400
C	3.88904300	-4.94330600	2.00081600
C	3.59231000	-3.81253500	1.21878000
C	4.26173800	-3.93615100	-0.16489300
C	5.10841300	-5.19851300	0.02905200
C	6.01652600	-5.77451100	-0.84742400
C	6.65596900	-6.96267900	-0.47501000
C	6.38520500	-7.55824900	0.76157000
C	5.47856200	-6.97469600	1.64922500
C	3.29730400	-5.09381700	3.25376300
C	2.44892300	-4.09697700	3.72375700
C	2.19375200	-2.92016300	2.98655100
C	2.76979600	-2.80452200	1.70626500
C	5.14883000	-2.74984200	-0.54122700
C	5.46557100	-2.48917400	-1.88380300
C	6.33744800	-1.46728200	-2.23307300
C	6.92252300	-0.66940100	-1.24057500
C	6.62161000	-0.91693700	0.10238200
C	5.74476900	-1.95157500	0.43594900
C	1.18311600	-3.26432200	-2.28860500

C	0.12347400	-2.37149200	-2.68827800
C	-0.88636400	-3.16399000	-3.29148800
N	-0.43657500	-4.48117400	-3.32977400
C	0.79039400	-4.57043700	-2.67649100
C	1.57782100	-5.67250400	-2.34908700
C	2.72839500	-5.45197900	-1.58939600
C	3.11990300	-4.16417500	-1.17387200
C	2.34943000	-3.06687200	-1.55767700
C	-0.08238800	-1.01176800	-2.48848300
C	-1.30715100	-0.43998900	-2.83718900
C	-2.30483600	-1.24194200	-3.42733100
C	-2.10373700	-2.60045200	-3.67850200
C	-1.80626300	4.80520100	-0.65549900
C	-1.58373800	3.56568200	-1.40201800
C	-2.38203400	2.55260200	-0.84200500
C	-3.14582700	3.06628700	0.38240700
C	-2.73675900	4.55497500	0.37171700
C	-3.15921600	5.59739100	1.18826000
C	-2.63213200	6.87870400	0.99327700
C	-1.69044400	7.11755100	-0.01184200
C	-1.27408100	6.08051700	-0.84725600
C	-0.76095000	3.29299200	-2.49386000
C	-0.71908900	1.99265700	-2.99475800
C	-1.51657700	0.97650200	-2.44421800
C	-2.38123700	1.27590400	-1.37849300
C	-4.65092100	2.85769500	0.16677000
C	-5.40418500	3.77113300	-0.58620300
C	-6.74543100	3.54402000	-0.85969300
C	-7.37611100	2.38371300	-0.38997600
C	-6.63949000	1.45832500	0.35506100
C	-5.29047000	1.70400700	0.62364300
O	7.75821300	0.31461500	-1.68163600
C	14.05742100	8.09536000	-0.83248500
C	13.17185400	7.09006900	-0.09243500
C	12.45356200	6.11791300	-1.03338400
C	11.56553300	5.10722200	-0.30204500
C	10.84760800	4.13650600	-1.24380100
C	9.96214900	3.12476300	-0.51031000
C	9.24663300	2.15873100	-1.45892400
C	8.37597800	1.15904600	-0.71538600
O	-8.69719100	2.25265100	-0.70641700
C	-17.69389400	-2.20958500	-0.97607300
C	-16.24722900	-2.29541600	-0.48381400
C	-15.40152600	-1.08649000	-0.89579000

C	-13.95188700	-1.16301300	-0.40834100
C	-13.10774600	0.04576200	-0.82178400
C	-11.65781500	-0.03257800	-0.33474100
C	-10.82069200	1.17925900	-0.75392000
C	-9.38434300	1.08636300	-0.26535900
H	-1.50095000	1.08830000	6.25986300
H	-3.36171900	2.77852500	5.04538000
H	-4.12167100	3.54019000	2.82717800
H	-1.18687200	1.08692900	0.86668400
H	0.52961600	-1.07491600	1.74448100
H	2.01399700	-2.34218600	5.58488600
H	0.51681800	-0.76871800	6.74554400
H	6.23103500	-5.30763300	-1.80431900
H	7.37116000	-7.42373200	-1.15032400
H	6.89049400	-8.47979900	1.03708500
H	5.27906200	-7.43397600	2.61371800
H	3.48485400	-5.97843300	3.85658000
H	1.95969400	-4.23712500	4.68143100
H	2.59281600	-1.91077400	1.11651900
H	5.00831500	-3.08721000	-2.66562400
H	6.57692500	-1.26207500	-3.27158300
H	7.05621600	-0.31632500	0.89241000
H	5.52305300	-2.13325800	1.48233500
H	-1.00566400	-5.27265800	-3.58572500
H	1.29772500	-6.68015100	-2.64276900
H	3.32620600	-6.30631700	-1.29474500
H	2.63850900	-2.06541800	-1.25569000
H	0.67672100	-0.40292600	-2.00581600
H	-3.25482100	-0.78636900	-3.69138600
H	-2.88594500	-3.20023200	-4.13523700
H	-3.89976200	5.43705900	1.96362700
H	-2.96274000	7.69561600	1.62848800
H	-1.28843200	8.11742200	-0.14942900
H	-0.55381600	6.26570200	-1.63954200
H	-0.14542400	4.07168900	-2.93612500
H	-0.05437100	1.74720300	-3.81791600
H	-2.99136700	0.48903400	-0.94456700
H	-4.93154800	4.67259500	-0.96205200
H	-7.32942900	4.25338700	-1.43743300
H	-7.09809300	0.55244100	0.73321200
H	-4.73305400	0.98068800	1.20973200
H	14.55868200	8.77811900	-0.13731600
H	14.83260100	7.58339100	-1.41564900
H	13.46704700	8.70218500	-1.52983400

H	12.42571000	7.62893000	0.50826000
H	13.78127800	6.51804300	0.62126200
H	13.19925700	5.57835700	-1.63569200
H	11.84272400	6.68913500	-1.74789000
H	10.82038100	5.64700200	0.30052300
H	12.17694800	4.53591400	0.41176600
H	11.59154300	3.59675900	-1.84731500
H	10.23374600	4.70639800	-1.95609500
H	9.21889900	3.66491100	0.09394300
H	10.57713700	2.55425600	0.20081000
H	9.98016200	1.60718800	-2.06045300
H	8.61758300	2.71745300	-2.16333200
H	7.60686000	1.67712000	-0.12365800
H	8.98123500	0.55625800	-0.02230000
H	-18.27616500	-3.08538000	-0.66850200
H	-18.19389200	-1.31864900	-0.57695000
H	-17.73490800	-2.14827600	-2.07042800
H	-15.78019100	-3.21176600	-0.87129800
H	-16.23581100	-2.38789200	0.61130400
H	-15.86786600	-0.16864900	-0.50846000
H	-15.41246000	-0.99270400	-1.99169000
H	-13.48616300	-2.08109200	-0.79561900
H	-13.94125100	-1.25625900	0.68753000
H	-13.57148100	0.96414900	-0.43386800
H	-13.11748500	0.13959100	-1.91724800
H	-11.19471700	-0.95149300	-0.72272300
H	-11.64829800	-0.12535000	0.76102100
H	-11.26712400	2.10119800	-0.36044200
H	-10.81441300	1.27404200	-1.84708800
H	-8.89413500	0.18725100	-0.66726900
H	-9.35008400	1.02262800	0.83244900

Syn-isomer：

C	1.53521600	-2.10065700	3.28161900
C	0.09839600	-2.26989400	3.35367300
C	-0.31051800	-1.77662800	4.62224000
N	0.81097300	-1.29979100	5.28664200
C	1.93240100	-1.47077600	4.48750700
C	3.26151600	-1.10280400	4.70299300
C	4.18313400	-1.39531100	3.70518800
C	3.82789100	-2.07562700	2.51740400
C	2.49424000	-2.42324600	2.31485500
C	-0.86256800	-2.75392600	2.46407900

C	-2.20717600	-2.78219300	2.84338600
C	-2.57890600	-2.32924900	4.12674700
C	-1.64606500	-1.81485400	5.02368500
C	-5.91411100	-4.59160400	-1.12434400
C	-5.04383500	-4.29261300	0.01515600
C	-4.42373200	-3.04949700	-0.20234200
C	-4.93202100	-2.40540600	-1.50274300
C	-5.85729600	-3.51716600	-2.03283800
C	-6.60556600	-3.55843900	-3.20263900
C	-7.40397000	-4.67712300	-3.46519200
C	-7.45572200	-5.74401400	-2.56319600
C	-6.71023000	-5.70753100	-1.38411400
C	-4.78813800	-5.01608800	1.17992200
C	-3.88501200	-4.50233500	2.10957200
C	-3.23054500	-3.28056900	1.88529400
C	-3.52389200	-2.54406800	0.72493500
C	-5.71750700	-1.13657700	-1.11797100
C	-7.07652900	-1.19106500	-0.77708500
C	-7.75585100	-0.05880500	-0.34766500
C	-7.08882400	1.16825100	-0.23997100
C	-5.73165200	1.24014300	-0.56951600
C	-5.06426200	0.09248900	-1.00183700
C	-1.53525600	-2.10073700	-3.28162400
C	-0.09843800	-2.26999300	-3.35367200
C	0.31048400	-1.77676700	-4.62225200
N	-0.81100500	-1.29995900	-5.28668000
C	-1.93243300	-1.47089200	-4.48753400
C	-3.26154300	-1.10291100	-4.70303200
C	-4.18316400	-1.39537000	-3.70521500
C	-3.82792800	-2.07564400	-2.51740500
C	-2.49428300	-2.42327800	-2.31484800
C	0.86252000	-2.75401000	-2.46406400
C	2.20712900	-2.78229600	-2.84336500
C	2.57886800	-2.32938300	-4.12673400
C	1.64603300	-1.81500800	-5.02369000
C	5.91401600	-4.59167600	1.12442400
C	5.04374800	-4.29269800	-0.01508600
C	4.42368200	-3.04955600	0.20237100
C	4.93198200	-2.40544000	1.50275600
C	5.85723000	-3.51720700	2.03288400
C	6.60550400	-3.55846300	3.20268400
C	7.40387700	-4.67716000	3.46527100
C	7.45559800	-5.74408200	2.56331000
C	6.71010400	-5.70761600	1.38422900

C	4.78803000	-5.01620400	-1.17982600
C	3.88491900	-4.50245800	-2.10949300
C	3.23048900	-3.28066400	-1.88525800
C	3.52385800	-2.54413100	-0.72492500
C	5.71749300	-1.13663600	1.11795600
C	7.07649700	-1.19116600	0.77700200
C	7.75583500	-0.05892400	0.34756100
C	7.08884500	1.16815700	0.23991600
C	5.73169200	1.24009000	0.56953200
C	5.06428400	0.09245400	1.00187200
O	-7.84227600	2.22346200	0.18649600
C	-9.65392500	11.72492300	2.90345400
C	-8.61081700	10.72246600	2.40394200
C	-9.17920500	9.31342100	2.20901500
C	-8.14299800	8.30281300	1.70918600
C	-8.71233000	6.89465500	1.51519900
C	-7.67451600	5.88539100	1.01526900
C	-8.25114700	4.47959200	0.82484900
C	-7.20894200	3.49045500	0.32900500
O	7.84231100	2.22334700	-0.18657600
C	9.65414500	11.72477900	-2.90351000
C	8.61102900	10.72235100	-2.40395500
C	9.17937800	9.31328500	-2.20907600
C	8.14316400	8.30270600	-1.70920600
C	8.71245700	6.89452700	-1.51526500
C	7.67463400	5.88529200	-1.01529400
C	8.25122700	4.47947100	-0.82492200
C	7.20901400	3.49036400	-0.32903700
H	0.80706200	-0.87139400	6.19849700
H	3.56905900	-0.59019100	5.61006400
H	5.20879000	-1.06749400	3.83327900
H	2.19426600	-2.93960100	1.41077700
H	-0.57297500	-3.11608700	1.48134300
H	-3.62802100	-2.36018000	4.40569000
H	-1.95452200	-1.44729600	5.99836900
H	-6.57840900	-2.73882100	-3.91186800
H	-7.98907200	-4.71483800	-4.37971800
H	-8.07989100	-6.60605800	-2.78133500
H	-6.74881100	-6.53553100	-0.68145000
H	-5.27424600	-5.97146200	1.35844100
H	-3.65604300	-5.06141500	3.01228200
H	-3.04525600	-1.58173200	0.57023300
H	-7.61100400	-2.13203900	-0.84911700
H	-8.80921500	-0.10053100	-0.08935000

H	-5.18716500	2.17416200	-0.49837800
H	-4.01319400	0.16568600	-1.26157800
H	-0.80707200	-0.87149700	-6.19850400
H	-3.56908200	-0.59032900	-5.61012200
H	-5.20881700	-1.06754500	-3.83331700
H	-2.19431500	-2.93960500	-1.41075200
H	0.57292000	-3.11614600	-1.48132000
H	3.62798400	-2.36032800	-4.40567200
H	1.95449600	-1.44748100	-5.99838400
H	6.57837300	-2.73882100	3.91188600
H	7.98898200	-4.71486100	4.37979600
H	8.07974400	-6.60613600	2.78147500
H	6.74866100	-6.53564000	0.68159100
H	5.27411000	-5.97159900	-1.35831300
H	3.65593200	-5.06156200	-3.01218300
H	3.04524900	-1.58177700	-0.57025500
H	7.61094400	-2.13215900	0.84899600
H	8.80918500	-0.10068200	0.08919300
H	5.18723300	2.17412900	0.49843500
H	4.01323300	0.16568400	1.26167000
H	-9.22205500	12.72344300	3.03425400
H	-10.48788300	11.81131900	2.19627100
H	-10.07097300	11.41195100	3.86843000
H	-7.77266800	10.67880500	3.11357500
H	-8.18651100	11.07542200	1.45348600
H	-10.01829400	9.35576800	1.49904300
H	-9.60421100	8.95899600	3.15963400
H	-7.30408500	8.26099400	2.41928200
H	-7.71853200	8.65746400	0.75849200
H	-9.55055100	6.93495500	0.80475800
H	-9.13591800	6.53860700	2.46532900
H	-6.83627900	5.84588300	1.72603400
H	-7.25177200	6.24162700	0.06457500
H	-9.08100100	4.50554500	0.10736400
H	-8.66464100	4.10944400	1.77144900
H	-6.37428100	3.41500000	1.04163300
H	-6.79449400	3.81434500	-0.63733700
H	9.22230200	12.72331600	-3.03427500
H	10.48814300	11.81113800	-2.19637000
H	10.07113200	11.41180500	-3.86851100
H	7.77284200	10.67872800	-3.11354600
H	8.18678500	11.07531100	-1.45347300
H	10.01850600	9.35559500	-1.49914700
H	9.60432300	8.95885700	-3.15972100

H	7.30421200	8.26092500	-2.41925800
H	7.71875900	8.65736000	-0.75848500
H	9.55071600	6.93478900	-0.80486700
H	9.13598400	6.53847600	-2.46542200
H	6.83635900	5.84582100	-1.72601600
H	7.25195100	6.24153100	-0.06457400
H	9.08111900	4.50538700	-0.10747900
H	8.66465900	4.10932000	-1.77154700
H	6.37431300	3.41494600	-1.04162300
H	6.79462600	3.81425500	0.63733100

Anti-isomer/I^-：

C	-0.40835900	-0.68869400	3.24961200
C	0.84294800	-1.37934000	3.55628000
C	0.74983900	-1.78408500	4.92259300
N	-0.46951500	-1.39693400	5.41626600
C	-1.19149900	-0.73765600	4.43215700
C	-2.47379800	-0.19663400	4.49747500
C	-2.96601100	0.42207900	3.35539300
C	-2.20537800	0.52548600	2.17204100
C	-0.92057000	-0.04130500	2.12093500
C	1.98652500	-1.69679100	2.83200700
C	3.05114400	-2.40118100	3.44915700
C	2.92444700	-2.74301300	4.82573100
C	1.79479000	-2.45447700	5.56597300
C	7.78459000	-3.62173600	0.44646700
C	6.65573400	-3.46385700	1.35371800
C	5.69936100	-2.61419200	0.75819300
C	6.14594100	-2.22856600	-0.66207400
C	7.52583700	-2.88895000	-0.73318200
C	8.45339800	-2.86534400	-1.76293000
C	9.65299400	-3.57324800	-1.60762000
C	9.91070500	-4.30334100	-0.44054000
C	8.97860500	-4.33445600	0.59601100
C	6.40312300	-3.99808800	2.62222500
C	5.22529800	-3.66314200	3.27207600
C	4.26614300	-2.77832100	2.70614400
C	4.52788300	-2.27664200	1.40986600
C	6.15812800	-0.72091300	-0.91328500
C	6.21790800	-0.23241700	-2.24140400
C	6.00477500	1.10154400	-2.53034600
C	5.70958200	2.00958500	-1.49432300
C	5.73978500	1.55244900	-0.15656200

C	5.97605400	0.20044800	0.11018800
C	2.91007600	-2.83157700	-2.52801800
C	1.56348700	-2.40877100	-2.80781700
C	0.84727000	-3.54746700	-3.25724500
N	1.74627800	-4.60133900	-3.34125300
C	2.99757100	-4.20158600	-2.87589000
C	4.18109800	-4.91182500	-2.64631100
C	5.22871100	-4.24381600	-2.00781400
C	5.12021500	-2.89906300	-1.59274700
C	3.94845500	-2.18847700	-1.87974400
C	0.92955100	-1.19980300	-2.61655900
C	-0.47041700	-1.13330200	-2.74054700
C	-1.18816500	-2.28244500	-3.14900100
C	-0.54198100	-3.48165700	-3.44965600
C	-1.68128800	3.40364000	0.34319500
C	-1.38947600	2.40306700	-0.65972000
C	-2.03185600	1.18915900	-0.30345800
C	-2.79209500	1.35189000	1.01597400
C	-2.51525100	2.82948400	1.33157000
C	-2.95263500	3.59557200	2.40451300
C	-2.55349100	4.93251600	2.48480700
C	-1.71567400	5.49966200	1.50852700
C	-1.27224700	4.74078900	0.43237000
C	-0.63002200	2.48786500	-1.83962500
C	-0.46018800	1.34319100	-2.59593400
C	-1.04016300	0.11299500	-2.20961700
C	-1.89805800	0.06387500	-1.08936600
C	-4.27261700	1.05030800	0.75929200
C	-5.14391200	2.04892500	0.29779900
C	-6.46083500	1.75729700	-0.02535700
C	-6.94764700	0.44617500	0.09497300
C	-6.08647000	-0.56466700	0.54339300
C	-4.76526900	-0.25360800	0.86676100
O	5.43144800	3.26521200	-1.87238800
C	-2.31403600	9.60780500	-0.93052400
C	-1.00717100	9.10094200	-0.31633000
C	-0.28919800	8.07623100	-1.20054200
C	0.99380400	7.52187100	-0.57384800
C	1.73425800	6.52875600	-1.47519900
C	2.94660200	5.88777700	-0.79370900
C	3.69240200	4.90845100	-1.70584900
C	4.81195000	4.19715900	-0.96255900
O	-8.24838000	0.26274400	-0.23857900
C	-16.79136900	-4.85882200	-1.58329600

C	-15.32085800	-4.92731600	-1.16362200
C	-14.61271600	-3.57086100	-1.24238300
C	-13.14047900	-3.62879000	-0.82396800
C	-12.43437800	-2.27194400	-0.90204100
C	-10.96248200	-2.33200000	-0.48142100
C	-10.26423800	-0.97051200	-0.55980300
C	-8.80723100	-1.04872800	-0.13588300
H	-0.79398400	-1.56543900	6.35745900
H	-3.07082600	-0.25649100	5.40230100
H	-3.96921500	0.83211500	3.37157900
H	-0.32561200	0.02730400	1.21757100
H	2.04765900	-1.39913400	1.79244400
H	3.74388500	-3.23186700	5.33533000
H	1.72851100	-2.73149300	6.61339800
H	8.26696300	-2.30321500	-2.67231300
H	10.39383600	-3.55097000	-2.40097900
H	10.84563300	-4.84609900	-0.34199600
H	9.17772400	-4.90166800	1.50046700
H	7.10904900	-4.67546500	3.09303400
H	5.04001400	-4.11244200	4.23911600
H	3.82762000	-1.60235000	0.93097800
H	6.37368400	-0.92885900	-3.05902900
H	6.01501000	1.46868300	-3.55070800
H	5.61655000	2.24097600	0.66857200
H	5.95661700	-0.12678000	1.14186300
H	1.50481500	-5.54658300	-3.60206700
H	4.28284300	-5.95752400	-2.91942900
H	6.14089100	-4.78983600	-1.79486800
H	3.81751700	-1.16640500	-1.54224100
H	1.48300300	-0.34158600	-2.25175300
H	-2.26770300	-2.22329700	-3.24797400
H	-1.10956000	-4.34278500	-3.78844400
H	-3.59548800	3.17107100	3.16792400
H	-2.89516800	5.54367800	3.31465100
H	-1.41411800	6.53828900	1.59731300
H	-0.61982600	5.17112900	-0.31854200
H	-0.16052800	3.42144200	-2.13195800
H	0.17925600	1.36454800	-3.47208900
H	-2.34233000	-0.88074900	-0.79122800
H	-4.78789500	3.06834700	0.19192400
H	-7.13826200	2.52956600	-0.37429400
H	-6.43340100	-1.58520400	0.65010100
H	-4.11481700	-1.04604200	1.22420100
H	-2.80374800	10.34248300	-0.28226500

H	-2.13354400	10.08601000	-1.90058400
H	-3.01821000	8.78280400	-1.09418300
H	-1.21417700	8.65250600	0.66626600
H	-0.33382100	9.94745800	-0.12489600
H	-0.05200000	8.53767900	-2.16972100
H	-0.97733600	7.24672900	-1.42256700
H	0.75401100	7.03360400	0.38229600
H	1.66733000	8.35354900	-0.32417400
H	2.05025300	7.03698200	-2.39678300
H	1.04321400	5.73279800	-1.79394400
H	2.60893100	5.35608600	0.10711000
H	3.63244900	6.67582100	-0.45204600
H	4.09925000	5.42802300	-2.58185200
H	2.99768900	4.14216000	-2.07125900
H	4.39449900	3.66604200	-0.10518200
H	5.58528100	4.89223600	-0.61514200
H	-17.27350700	-5.84042300	-1.51800600
H	-17.35237900	-4.16745600	-0.94283000
H	-16.89038300	-4.50565400	-2.61693500
H	-14.78948200	-5.64955900	-1.79926800
H	-15.24823700	-5.31350000	-0.13718300
H	-15.14338500	-2.84699800	-0.60669900
H	-14.68433300	-3.18299800	-2.26910800
H	-12.60969700	-4.35212600	-1.46026600
H	-13.06932200	-4.01697800	0.20266900
H	-12.96360800	-1.54812100	-0.26596800
H	-12.50269100	-1.88320100	-1.92813100
H	-10.43269800	-3.05483400	-1.11885800
H	-10.89489200	-2.72155800	0.54476400
H	-10.77889800	-0.24459500	0.08187100
H	-10.31332200	-0.57856600	-1.58332900
H	-8.24789400	-1.74065000	-0.78184700
H	-8.72007200	-1.40738500	0.89973000
I	2.38625900	1.37584200	0.08060700

Syn-isomer/I^-：

C	1.30935300	-2.52510400	3.34450700
C	-0.12767900	-2.70186500	3.43396700
C	-0.50698500	-2.31198900	4.75484000
N	0.61428200	-1.86685300	5.40994600
C	1.72085900	-1.95100400	4.57078200
C	3.03149200	-1.51895500	4.77027000
C	3.93243200	-1.71661200	3.72947300

C	3.57875500	-2.38971300	2.53987800
C	2.25119200	-2.78693400	2.34955200
C	-1.10924000	-3.04921400	2.52045300
C	-2.45563200	-3.09155200	2.93454700
C	-2.78795600	-2.81879000	4.28905000
C	-1.83455100	-2.39916600	5.20049000
C	-6.41696600	-4.07648100	-1.01265600
C	-5.51155700	-3.95013500	0.10959500
C	-4.55106600	-2.94528000	-0.17641400
C	-4.92640000	-2.21800100	-1.47873000
C	-6.08441800	-3.10053600	-1.98255800
C	-6.82507500	-3.02659200	-3.15676300
C	-7.88072500	-3.92169300	-3.35587200
C	-8.20642600	-4.88735800	-2.39122000
C	-7.47704200	-4.97039800	-1.21101100
C	-5.50352800	-4.62755600	1.33648100
C	-4.52742900	-4.30908900	2.26517400
C	-3.51493400	-3.36657600	1.96227700
C	-3.53816100	-2.67842900	0.72742200
C	-5.41532400	-0.81729800	-1.04654100
C	-6.75093700	-0.57930400	-0.69075000
C	-7.15364800	0.66482000	-0.22704600
C	-6.22228700	1.70667800	-0.09140200
C	-4.88057400	1.47671400	-0.43086700
C	-4.49186300	0.22443700	-0.90212200
C	-1.58348200	-2.39531100	-3.35628700
C	-0.16138300	-2.65887100	-3.44614200
C	0.24540100	-2.27192000	-4.75437200
N	-0.84564500	-1.75384200	-5.41066600
C	-1.95508000	-1.77915200	-4.57595400
C	-3.23191300	-1.24682800	-4.76464300
C	-4.13560400	-1.37897400	-3.71915300
C	-3.82789200	-2.08575000	-2.53343700
C	-2.53551400	-2.58813700	-2.35545800
C	0.79621900	-3.05914400	-2.52668800
C	2.14927000	-3.16627100	-2.93678700
C	2.49888400	-2.89862800	-4.28529200
C	1.56978300	-2.42032000	-5.19422700
C	5.99190600	-4.58604700	0.99271500
C	5.11446900	-4.34864800	-0.13357900
C	4.24485000	-3.26960400	0.17439000
C	4.67257900	-2.61181700	1.49554900
C	5.73053300	-3.61472800	1.98928700
C	6.44611700	-3.64764900	3.18008000

C	7.41323500	-4.64039300	3.36685500
C	7.67380100	-5.59754900	2.37392900
C	6.96498400	-5.57676300	1.17850100
C	5.05589400	-4.98587200	-1.38123400
C	4.11836200	-4.55554700	-2.30458900
C	3.18581900	-3.53943500	-1.97605400
C	3.26737800	-2.88796400	-0.72469800
C	5.30446700	-1.25925100	1.09521900
C	6.66891100	-1.13679200	0.79476600
C	7.19581900	0.06964000	0.35607700
C	6.36372600	1.18825300	0.18975300
C	4.99439100	1.07463400	0.47598200
C	4.48102100	-0.14017600	0.92342300
O	-6.71145600	2.88384300	0.36661100
C	-6.39809300	12.48991300	3.30564200
C	-5.59842300	11.29522100	2.77981500
C	-6.46145700	10.04873000	2.55839000
C	-5.67056000	8.84743600	2.03180800
C	-6.53499400	7.60261900	1.81078700
C	-5.74246400	6.40244300	1.28314100
C	-6.61508100	5.16229200	1.06430100
C	-5.81317300	3.98323900	0.53968100
O	6.96934500	2.31892900	-0.24415700
C	7.57023200	11.87023700	-3.31519800
C	6.65543900	10.75595500	-2.80063200
C	7.40288900	9.44654600	-2.52796100
C	6.49588900	8.32465200	-2.01352300
C	7.24461800	7.01636800	-1.74245600
C	6.33538800	5.89484400	-1.23015000
C	7.09216300	4.58957800	-0.96374600
C	6.17421100	3.48834300	-0.46078800
H	0.62813000	-1.49840500	6.35016600
H	3.33677500	-1.02125800	5.68536200
H	4.93550300	-1.31939800	3.82889900
H	1.94943200	-3.28016600	1.43464800
H	-0.85399600	-3.28348900	1.49415600
H	-3.82971500	-2.86222700	4.58921200
H	-2.11027000	-2.12378900	6.21350300
H	-6.60441300	-2.29137000	-3.91969800
H	-8.46038000	-3.86454400	-4.27214400
H	-9.03012200	-5.57116200	-2.57058900
H	-7.71835200	-5.71823800	-0.46170900
H	-6.25194200	-5.38189200	1.55846600
H	-4.49875200	-4.82102200	3.22197200

H	-2.79538700	-1.90914300	0.53612900
H	-7.48658800	-1.37137200	-0.78013900
H	-8.18762300	0.85795800	0.03875800
H	-4.13766400	2.25925700	-0.33751500
H	-3.44848200	0.06698500	-1.15858900
H	-0.83223900	-1.36927700	-6.34444000
H	-3.50183600	-0.71728100	-5.67289500
H	-5.10208300	-0.89809000	-3.80612900
H	-2.26703900	-3.10675600	-1.44418000
H	0.52167300	-3.33458100	-1.51597500
H	3.53796200	-2.99045900	-4.58295200
H	1.86469700	-2.14444400	-6.20181100
H	6.27033100	-2.92218000	3.96416000
H	7.97434900	-4.66812400	4.29595300
H	8.42926600	-6.35800600	2.54468100
H	7.15381100	-6.31929000	0.40911400
H	5.73461400	-5.79811800	-1.62201800
H	4.04754400	-5.03968000	-3.27350000
H	2.59929900	-2.05802300	-0.51788200
H	7.32952300	-1.98964200	0.90685900
H	8.25221700	0.17330400	0.13178400
H	4.32605100	1.91860000	0.35786400
H	3.41834900	-0.20819000	1.13586200
H	-5.75845400	13.36677800	3.45490200
H	-7.19312300	12.77145100	2.60452500
H	-6.87273800	12.25477800	4.26605900
H	-4.78984800	11.05417200	3.48422800
H	-5.10803600	11.56738600	1.83460100
H	-7.27108000	10.28851100	1.85362800
H	-6.95295700	9.77496600	3.50352300
H	-4.86106400	8.60750000	2.73678400
H	-5.17948200	9.12142400	1.08657400
H	-7.34407000	7.84088200	1.10562800
H	-7.02542200	7.32642700	2.75522600
H	-4.93352800	6.16349900	1.98876300
H	-5.25251900	6.67893500	0.33828800
H	-7.41867400	5.38684900	0.35193000
H	-7.09871400	4.86968800	2.00464900
H	-5.01879700	3.70303300	1.24573400
H	-5.34046600	4.22788000	-0.42199600
H	7.01165100	12.79404300	-3.50195700
H	8.36045900	12.09825700	-2.58962600
H	8.05756400	11.57859700	-4.25351600
H	5.85515800	10.56961900	-3.53065700

H	6.15612700	11.08544600	-1.87862900
H	8.20366400	9.63120900	-1.79698500
H	7.90368800	9.11583200	-3.44971200
H	5.69503200	8.14034300	-2.74462500
H	5.99578000	8.65513300	-1.09138100
H	8.04390400	7.19833500	-1.00989300
H	7.74512700	6.68490100	-2.66353900
H	5.53569000	5.71343700	-1.96291200
H	5.83606400	6.22564200	-0.30795600
H	7.88326500	4.75596800	-0.22204300
H	7.58593300	4.24528000	-1.88103400
H	5.38679300	3.26746500	-1.19496200
H	5.68753000	3.78235900	0.47980400
I	0.05615000	-0.54910100	-0.10404700

12. References

[1] Frisch, M. J., et al. (2016). Gaussian 16 Rev. A.03. Wallingford, CT.

[2] S. F. Boys, F. Bernardi, *Mol. Phys.* 1970, **19**, 553−566.

[3] X. B. Yang, B. X. Yang, J. F. Ge, Y. J. Xu, Q. F. Xu, J. Liang and J. M. Lu, *J Org Lett*, 2011, **13**, 2710-2713.