Supporting Information

for

9,10-Azaboraphenanthrene-Based Small Molecules and Conjugated Polymers: Synthesis and Their Application in Chemodosimeters for the Ratiometric Detection of Fluoride Ions

Weidong Zhang,[a] Guoping Li,[a] Letian Xu,[a] Yue Zhuo,[a] Wenming Wan,[b] Ni Yan[c] and Gang He*[,a]

[a]Frontier Institute of Science and Technology jointly with School of Science, State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi'an Key Laboratory of Sustainable Energy Materials Chemistry, Xi'an Jiaotong University, Xi'an, Shaanxi 710054, China.. E-mail: ganghe@mail.xjtu.edu.cn
[b]Centre for Bioengineering and Biotechnology, China University of Petroleum (East China), Qingdao, Shandong 266580, China
[c]Polymer Materials & Engineering Department and Institute of Polymer Materials, School of Materials Science & Engineering, Chang'an University, Xi'an, Shaanxi 710064, China

Contents

1. Materials and instrumentation

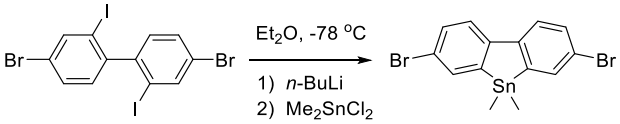
General. All reactions were performed using standard Schlenk and glovebox (Vigor) techniques under argon atmosphere. Et_2O, THF, hexanes and toluene were distilled from sodium/benzophenone prior to use. Trimethyltin chloride (99%), 4-methylphenylboronic acid (**7**) (98%), tetrakis(triphenylphosphine) palladium ($Pd(Ph_3P)_4$) (99%), potassium carbonate (99%), and were purchased from Energy Chemical Inc. Dimethyltin dichloride (Me_2SnCl_2) (99%) purchased from TCI. Phenylborondichloride ($PhBCl_2$) were obtained from Sigma-Aldrich. (3-hexylthiophene-2,5-diyl)bis(tributylstannane) (**10**) were prepared according to literature procedures,[1] 2,2'-(9,9-didecyl-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (**9**) were prepared according to literature procedures.[2] Azides were prepared according to literature procedures.[3] Unless otherwise indicated, all other reagents and solvents were used as commercially available without further purification. Column chromatographic purification of products was accomplished using 200-300 mesh silica gel.

NMR spectra were measured on a Bruker Avance-400 spectrometer in the solvents indicated; chemical shifts are reported in units (ppm) by assigning TMS resonance in the ^1H spectrum as 7.26 ppm, $CDCl_3$ resonance in the ^{13}C spectrum as 77.0 ppm. Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). UV-vis measurements were performed using DH-2000-BAL Scan spectrophotometer. Fluorescence measurements were conducted on an FLS920 system. Single crystal X-ray diffraction analysis was carried out on a Bruker Apex Duo instrument. The cyclic voltammetry (CV) were measured using a CHI660E B157216 set up. GPC measurements were made using a GPC 270 Max instrument equipped with a Viscotek VE 2001 plus autosampler, three μ-Styragel columns, and a Viscotek VE 3580 refractive index (RI) detector. The columns were calibrated using polystyrene standards. The average molecular weight of **P1** and **P2** were performed at 35 °C using THF as the eluent at a flow rate of 1.0 mL min^{-1}. High-resolution mass spectra

(HRMS) were collected on a Bruker maXisUHR-TOFmass spectrometer in an ESI positive mode for **2**, **5**, and **8** and APCI mode for **6**. Elemental analysis was conducted on a machine of Euro Vector EA3000.

2. Experimental procedures and data

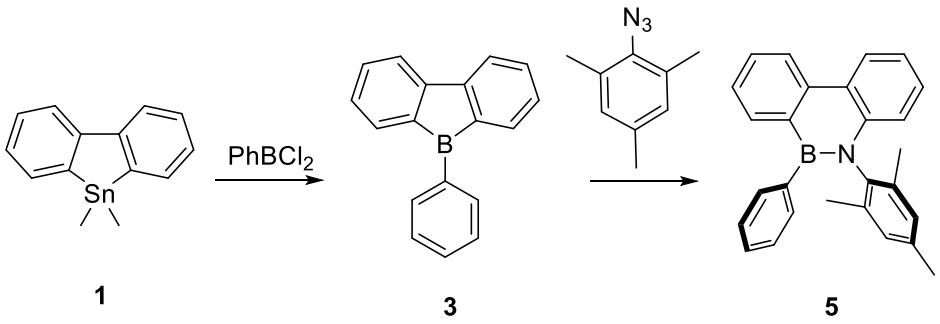
2.1 Synthesis of 4,4-dimethyl-4H-stannolo[3,2-b:4,5-b']dithiophene (2):



2

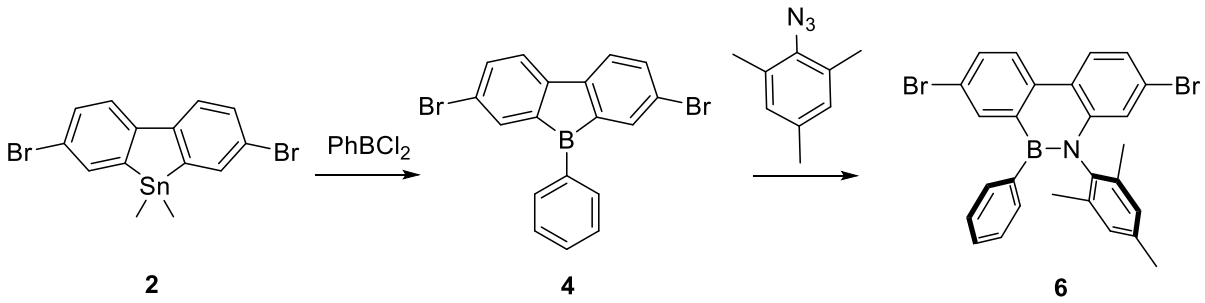
To a solution of 4,4'-dibromo-2,2'-diiodo-1,1'-biphenyl (1.685 g, 3.0 mmol) in Et_2O (30 mL) at -78 °C was added dropwise a solution of *n*-BuLi (2.5 M in hexanes, 2.5 mL, 6.3 mmol) via syringe. After the reaction mixture was warmed to room temperature, the solution was stirred for another 3 h. A solution of Me_2SnCl_2 (0.71 g, 3.2 mmol) in 15 mL Et_2O was then added dropwise at -78 °C via syringe, and the mixture was warmed to room temperature and stirred overnight. The solvent was removed under reduced pressure and the product was extracted with 60 mL hexanes three times, and the solution was filtered through Celite. The solvent was removed from the filtrate to give a light brown solid. This product was recrystallized from hexanes at -35 °C to give **2** as yellow crystals. Yield: 0.963 g (70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73-7.76 (m, 4H, Ar*H*), 7.50 (dd, *J* = 8.4 Hz, 2Hz, Ar*H*), 0.58 (s, 6H, Sn(CH_3)$_2$); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.0, 143.6, 138.6, 132.1, 124.0, 122.8 (Ar-*C*), -8.2 (Sn(*C*H_3)$_2$), HRMS (ESI) *m*/*z*: $[M + H]^+$ calcd for $C_{14}H_{13}Br_2Sn$, 458.8401, found, 458.8386. Mp (°C): 136.8-138.7.

2.2 Synthesis of 5-mesityl-6-phenyl-5,6-dihydrodibenzo[c,e][1,2]azaborinine (5):



To a solution of **1** (0.903 g, 3.0 mmol) in a 30 mL toluene at -78 °C was added dropwise a solution of $PhBCl_2$ (0.476 g, 3.0 mmol) in toluene (5 mL) via syringe. Then the mixture was slowly warmed to room temperature and stirred overnight. After $MesN_3$ (3.6 mmol) was added dropwise at room temperature stirred for 12 h. The solvent was removed under reduced pressure, the product was purified via column chromatography (silica gel, Petroleum ether/ ethylcetate = 50 :1) afforded 0.560 g (50 %) of the white title compound. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 7.6 Hz, 2H, Ar*H*), 7.89 (d, *J* = 7.6 Hz, 1H, Ar*H*), 7.76-7.81 (m, 1H, Ar*H*), 7.46 (t, *J* = 14.4 Hz, 7.2 Hz, 1H, Ar*H*), 7.27-7.32 (m, 4H, Ar*H*), 7.19-7.23 (m, *3*H, Ar*H*), 6.86 (s, 2H, Ar*H*), 6.79-6.81 (m, 1H, Ar*H*), 2.27 (s, 3H, -CH_3), 1.88 (s, 6H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 139.2, 139.1, 137.5, 136.4, 134.9, 132.5, 131.1, 129.1, 128.3, 127.2, 126.7, 126.0, 124.5, 124.1, 121.9, 121.8, 117.1 (Ar-*C*), 21.0, 18.0 (Mes-CH_3); ^{11}B NMR (193 MHz, $CDCl_3$) δ 39.1 (bs). HRMS (ESI) *m*/*z*: $[M + H]^+$ calcd for $C_{27}H_{25}BN$, 374.2075, found, 374.2063. Anal. Calcd. For $C_{27}H_{24}BN$: C, 86.87; H, 6.48; N, 3.75. Found : C, 85.84; H, 6.37; N, 3.73. UV/vis (in THF): λ_{max} (ε) = 317 nm (1.30×10^4 M^{-1} cm^{-1}). Fluorescence emission (in THF) (λ_{ex} = 300 nm): λ_{emis} = 355 nm. (Quantum yields, Φ = 0.52). Mp (°C): 204.6-205.4.

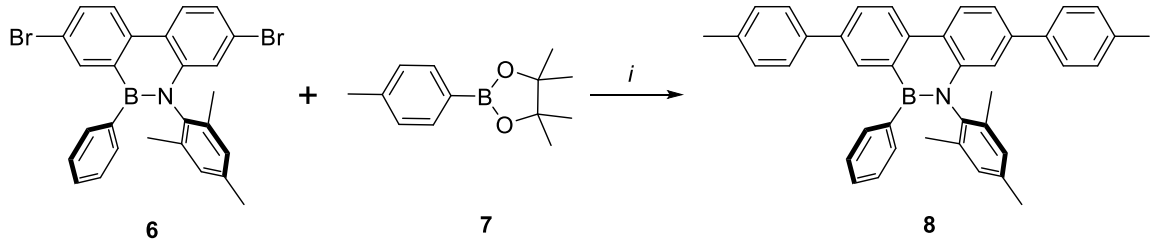
2.3 Synthesis of 3,8-dibromo-5-mesityl-6-phenyl-5,6-dihydrodibenzo[c,e][1,2] azabor-inine (6):



2 **4** **6**

To a solution of **2** (1.376 g, 3.0 mmol) in a 30 mL toluene at -78 °C was added dropwise a solution of $PhBCl_2$ (0.476 g, 3.0 mmol) in toluene (5 mL) via syringe. Then the mixture was slowly warmed to room temperature and stirred overnight. After $MesN_3$ (3.6 mmol) was added dropwise at 40 °C, and stirred 12 h. The solvent was removed under reduced pressure, the product was purified via column chromatography (silica gel, Petroleum ether/ ethyl acetate = 50 :1) afforded 1.131 g (71 %) of the white title compound. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 (dd, *J* = 8.8 Hz, 4.4 Hz, 2H, Ar*H*), 7.97 (d, *J* = 2.4 Hz, 1H, Ar*H*), 7.86 (dd, *J* = 8.8 Hz, 2.4 Hz, 1H, Ar*H*), 7.43 (dd, *J* = 8.8 Hz, 2.0 Hz, 1H, Ar*H*), 7.20-7.25 (m, 5H, Ar*H*), 6.93 (d, *J* = 2.0 Hz, 1H, Ar*H*), 6.86 (s, 2H, Ar*H*), 2.28 (s, 3H, -CH_3), 1.86 (s, 6H, -CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 139.6, 138.2, 137.1, 137.0, 134.5, 134.4, 132.3, 129.4, 127.7, 127.0, 125.5, 125.3, 123.8, 122.8, 122.8, 121.1, 119.9 (Ar-*C*), 21.0, 18.0 (Mes-CH_3); ^{11}B NMR (193 MHz, $CDCl_3$) δ 39.2 (bs). HRMS (APCI) *m*/*z*: $[M]^+$ calcd for $C_{27}H_{22}Br_2BN$, 531.0192, found, 531.0187. Anal. Calcd. For $C_{27}H_{22}BBr_2BN$: C, 61.06; H, 4.18; N, 2.64. Found: C, 60.92; H, 4.18; N, 2.57. UV/vis (in THF): λ_{max} (ε) = 324 nm (1.07×10^4 M^{-1} cm^{-1}). Mp (°C): 218.3-220.6.

2.4 Synthesis of 5-mesityl-6-phenyl-3,8-di-p-tolyl-5,6-dihydrodibenzo[c,e][1,2] azabor-inine (8):



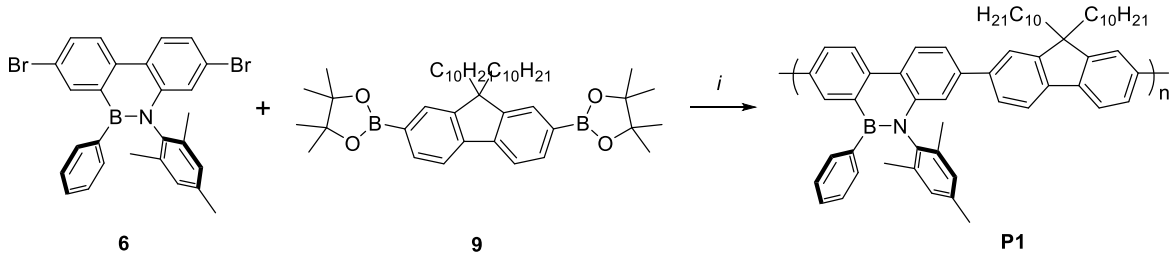
6 **7** **8**

i) $Pd(PPh_3)_4$, 5 mol%, Aliquant336, 10 mol%, K_2CO_3 (2M),Toluene

Monomer **6** (0.212g, 0.4 mmol), monomer **7** (0.17g, 0.8 mmol), $Pd(PPh_3)_4$ (24 mg, 5 mmol%), Aliquant336 (16 mg, 10 mmol%) and Ar_2-sparged aqueous potassium carbonate (2.0 M, 3.6 mL, 2.0 mmol) were dissolved in 8 mL of toluene in a Schlenk flask. The reaction mixture was stirred for 48 h at 110 °C. The reaction mixture was then cooled to room temperature, the solvent was removed in vacuo, the product was purified via column chromatography (silica gel, Petroleum ether/ ethyl acetate = 50 :1) afforded the white title compound, recrystallized from hexanes and CH_2Cl_2 at -30 °C to give **8** as white crystals (0.115g, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (dd, *J* = 8.4 Hz, 5.2 Hz, 2H, Ar*H*), 8.12 (d, *J* = 2.0 Hz, 1H, Ar*H*), 8.02 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H, Ar*H*), 7.55 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H, Ar*H*), 7.51 (d, *J* = 8.4 Hz, 1H, Ar*H*), 7.36 (d, *J* = 8.0 Hz, 2H, Ar*H*), 7.29-7.31 (m, 2H, Ar*H*), 7.20-7.25 (m, 7H, Ar*H*), 7.01 (d, *J* = 2.0 Hz, 1H, Ar*H*), 6.85 (s, 2H, Ar*H*), 2.39 (s, 3H, C*H*$_3$), 2.37 (s, 3H, C*H*$_3$), 2.23 (s, 3H, C*H*$_3$), 1.93 (s, 6H, C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 140.4, 139.0, 138.1, 137.2, 137.0, 136.4, 135.5, 134.8, 132.5, 130.0, 129.5, 129.4, 129.2, 127.2, 127.1, 126.8, 124.5, 123.2, 122.5, 120.9, 115.2 (Ar-*C*), 21.1, 21.0, 18.1 (CH_3-C); ^{11}B NMR (193 MHz, $CDCl_3$) δ 40.5 (bs).

HRMS (ESI) *m*/*z*: $[M + H]^+$ calcd for $C_{41}H_{37}BN$, 554.3014, found, 554.3014. UV/vis (in THF): λ_{max} (ε) = 320 nm ($3.36 \times 10^4\ M^{-1}\ cm^{-1}$). Fluorescence emission (in THF) (λ_{ex} = 300 nm): λ_{emis} = 391 nm (Quantum yields, Φ = 0.77). Mp (°C): 242.3-243.6.

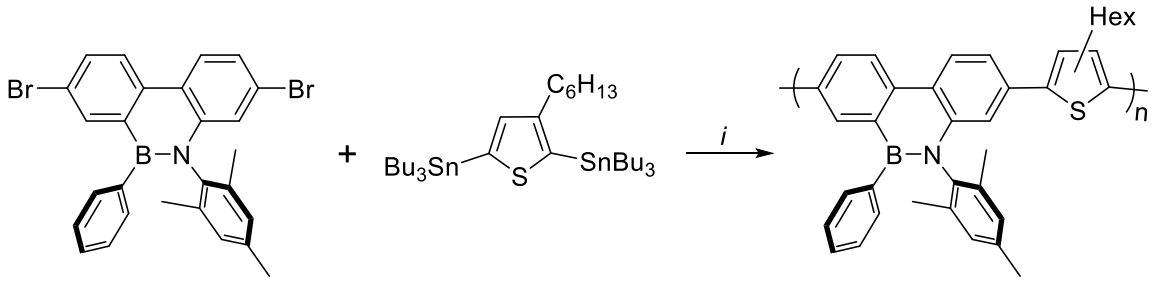
2.5 Synthesis of P1:



i) $Pd(PPh_3)_4$, 5 mol%, Aliquant336, 10 mol%, K_2CO_3 (2M),Toluene

Monomer **6** (0.212g, 0.4 mmol), monomer **9** (0.28 g, 0.4 mmol), $Pd(PPh_3)_4$ (24 mg, 5 mmol%), Aliquant336 (16 mg, 10 mmol%) and Ar_2-sparged aqueous potassium carbonate (2.0 M, 3.6 mL, 2.0 mmol) were dissolved in 8 mL of toluene in a Schlenk flask. The reaction mixture was stirred for 48 h at 110 °C. The reaction mixture was then cooled to room temperature, the solvent was removed in vacuo, and the residue was dissolved in 1 mL $CHCl_3$, then reprecipitated in MeOH (200 mL), the precipitate was purified by Soxhlet extraction using acetone to remove the residual monomer and then extracted with chloroform. ^1H NMR (400 MHz, $CDCl_3$): δ 8.69, 8.53, 8.23, 8.13, 7.78, 7.70, 7.69, 7.59, 7.48, 7.39, 7.14, 6.92 (Ar*H*), 2.43, 2.31 (Mes-*H*), 2.08, 2.00, 1.98, 1.96, 1.26, 1.25, 1.21, 1.16, 1.05, 0.86, 0.84, 0.83, 0.81, 0.69 (octyl)). UV/vis (in THF): λ_{max} (ε) = 379 nm ($3.57 \times 10^4\ M^{-1}\ cm^{-1}$). Fluorescence emission (in THF) (λ_{ex} = 350 nm): λ_{emis} = 414 nm (Quantum yields, Φ = 0.88). *M*n = 6.17 kg/mol, *M*w = 9.40 kg/mol, PDI = 1.53 by GPC.

2.6 Synthesis of P2:



6 **10** **P2**

i) P-(O-tolyl), $Pd_2(dba)_3$, Toluene

Monomer **6** (0.425g, 0.8 mmol), monomer **10** (0.0.597 g, 0.8 mmol), $Pd_2(dba)_3$ (11.0 mg, 0.012mmol) and P(*o*-Tolyl)$_3$ (18.4 mg, 0.061 mmol) were dissolved in 8 mL of toluene in a Schlenk flask. The reaction mixture was stirred for 48 h at 110 °C. The reaction mixture was then cooled to room temperature, the solvent was removed in vacuo, and the residue was dissolved in 1 mL $CHCl_3$, then reprecipitated in MeOH (200 mL), the precipitate was purified by Soxhlet extraction using acetone to remove the residual monomer and then extracted with chloroform. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52, 8.10, 7.98, 7.95, 7.54, 7.28, 7.23, 7.22, 7.19, 7.00, 6.98, (Ar*H*), 6.88 (s, thienyl-*H*), 6.83 (s, thienyl-*H*), 2.59, 2.57, 2.28 (hexyl), 2.25, 1.92, (Mes-*H*), 1.58, 1.50, 1.43, 1.21-1.37, 0.83-0.94 (hexyl). UV/vis (in THF): λ_{max} (ε) = 398 nm (3.07×10^4 M^{-1} cm^{-1}). Fluorescence emission (in THF) (λ_{ex} = 365 nm): λ_{emis} = 458 nm (Quantum yields, Φ = 0.57). *M*n = 6.08 kg/mol, *M*w = 8.04 kg/mol, PDI = 1.37 by GPC.

3. Proposed mechanism for ring expansion of borole with azide

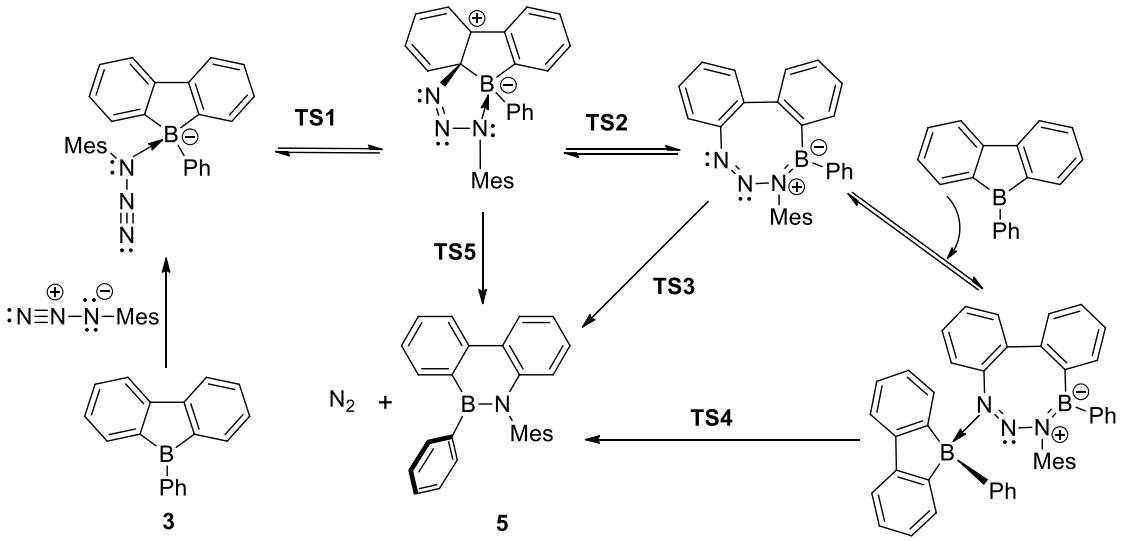


Figure S1. Proposed mechanism for ring expansion of borole with azide.

4. DFT computations

All calculations were carried out with the GAUSSIAN 09 program package.[4] The geometries for the ground state of compounds 5, 8, P1, P2, 5- F, 5- F', 8- F, 8- F', P1- F, P1- F', P2- F, P2- F' were optimized at the B3LYP level with the 6-31G* basis set.[5-7]

The simulated UV–Vis spectra for optimized molecules were performed at the time dependent density functional theory (TD-DFT)[8,9] at the ground-state equilibrium geometries were determined using the B3LYP,[5-7] in association with the 6-31G* basis set.

It should be pointed out that the structures of all stationary points were fully optimized, and frequency calculations were performed at the same level. The frequency calculations confirmed the nature of all revealed equilibrium geometries: there were no imaginary frequencies.

5. Single-crystal X-ray structure determination

X-ray Crystallography. Crystals of appropriate quality for X-ray diffraction studies were removed from a vial (in a glove box) and immediately covered with a thin layer of hydrocarbon oil (Paratone-N). A suitable crystal was then selected, attached to a glass fiber, and quickly placed in a glass vial. All data were collected using a Bruker APEX II CCD detector/D8 diffractometer using Mo/Cu Kα radiation. The data were corrected for absorption through Gaussian integration from indexing of the crystal faces. Structures were solved using the direct methods programs SHELXS-97, and refinements were completed using the program SHELXL-97.[10]

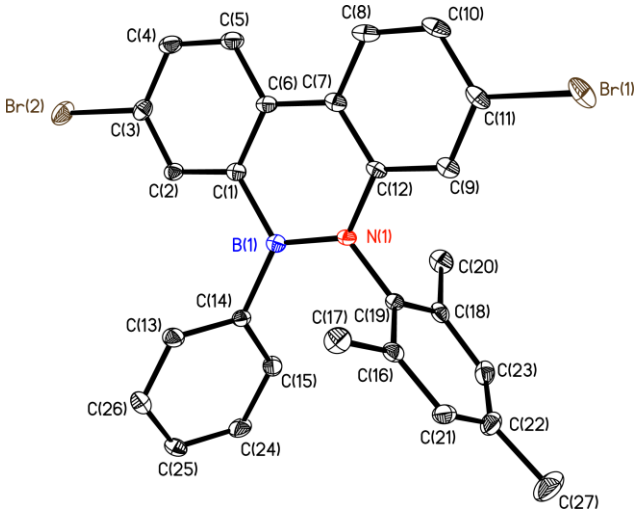


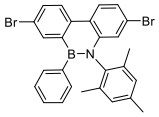
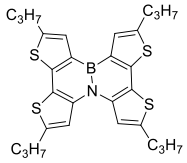
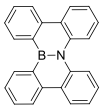
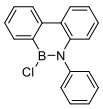
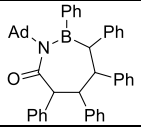
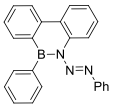
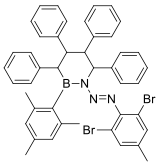
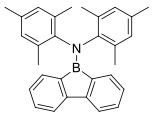
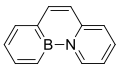
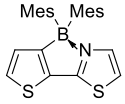
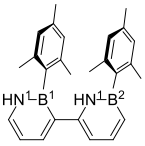
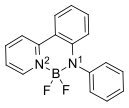
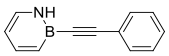
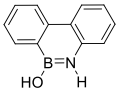
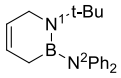
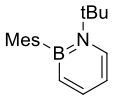
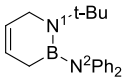
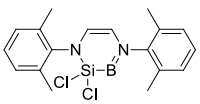
Figure S2. Molecular Structure of **6** (CCDC 1818909) with thermal ellipsoids presented at a 50% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å): N(1)—C(12), 1.412(4); N(1)—B(1), 1.414(5); N(1)—C(19), 1.452(5); B(1)—C(1), 1.551(6); B(1)—C(14), 1.576(5). Bond angles (deg): C(12)—N(1)—B(1), 123.2(3); C(12)—N(1)—C(19), 116.1(3); B(1)—N(1)—C(19), 120.7(3); N(1)—B(1)—C(1), 116.0(3); N(1)—B(1)—C(14), 121.8(3); C(1)—B(1)—C(14), 122.2(3).

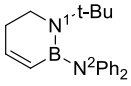
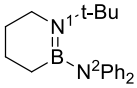
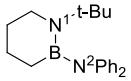
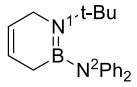
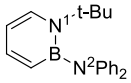
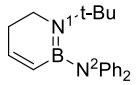
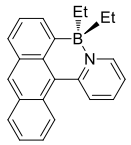
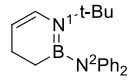
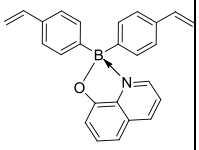
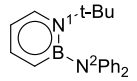
Table S1. Crystallographic experimental details for compound **6** (CCDC 1818909).

Empirical formula	$C_{27}H_{22}BBr_2N$
Formula weight	531.08
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 11.2690(4) Å α = 90 deg.
	b = 7.3358(3) Å β = 101.4180(10) deg.
	c = 14.2605(5) Å γ = 90 deg.
Volume	1155.54(7) Å^3
Z, Calculated density	2, 1.526 Mg/m^3
Absorption coefficient	3.522 mm^-1
F(000)	532
Crystal size	0.723 x 0.246 x 0.213 mm
Theta range for data collection	2.111 to 26.415 deg.
Limiting indices	-14<=h<=14, -9<=k<=9, -17<=l<=17
Reflections collected / unique	28928 / 4728 [R(int) = 0.0361]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4728 / 1 / 283
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0646
R indices (all data)	R1 = 0.0304, wR2 = 0.0664
Extinction coefficient	n/a
Largest diff. peak and hole	0.608 d -0.865 e. Å^-3

6. Comparison of bond distances in different BN-containing heterocycles

Table S2 Comparison of BN bond distances in different BN-containing heterocycles

	Structure	bond lengths		Structure	bond lengths
1		**1.414(5) This work**	**15**		1.474(6)[11]
2		1.426(3)[12]	**16**		1.402(3)[13]
3		1.498(2)[14]	**17**		1.426(3)[13]
4		1.443(3)[15]	**18**		1.442(3)[16]
5		1.491(2)[17]	**19**		1.667(3)[18]
6		B1–N1 1.4281(16), B2–N2 1.4253(15)[19]	**20**		N(1)-B, 1.498(3), N(2)-B, 1.598(3)[20]
7		1.427(5)[21]	**21**		1.414(4)[22]
8		N(1)-B, 1.4079(18), N(2)-B, 1.4780(17)[23]	**22**		1.447(2)[24]
9		N(1)-B, 1.417(3), N(2)-B, 1.480(3)[23]	**23**		1.4128(18)[25]

10		N(1)-B, 1.4075(19), N(2)-B, 1.4828(19)[23]	**24**		N(1)-B, 1.403(2), N(2)-B, 1.488(2)[23]
11		N(1)-B, 1.403(2), N(2)-B, 1.488(2)[23]	**25**		N(1)-B, 1.405(2) N(2)-B, 1.478(2)[23]
12		N(1)-B, 1.4460(17), N(2)-B, 1.4856(16)[23]	**26**		N(1)-B, 1.407(2) N(2)-B, 1.483(2)[23]
13		1.685(3)[26]	**27**		N(1)-B, 1.417(3) N(2)-B, 1.480(3)[23]
14		1.637(2)[27]	**26**		N(1)-B, 1.446(2) N(2)-B, 1.486(2)[23]

7. GPC data for P1 and P2

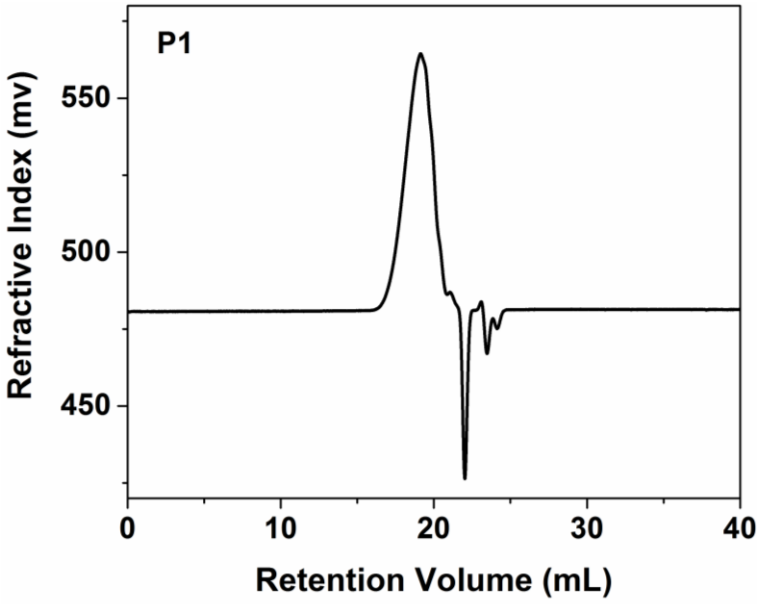


Figure S3. GPC of **P1** with THF as an eluent at 1 mL/min.

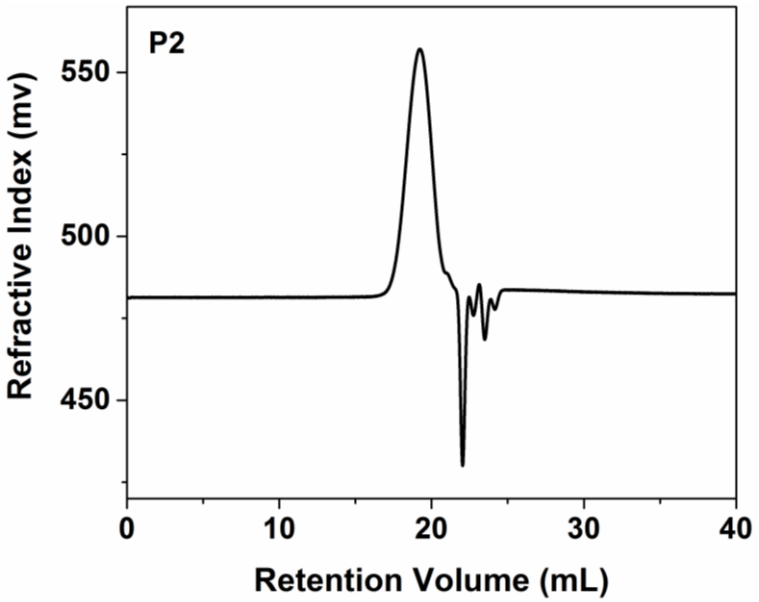


Figure S4. GPC of **P2** with THF as an eluent at 1 mL/min.

8. The UV-vis and excitation and emission spectra

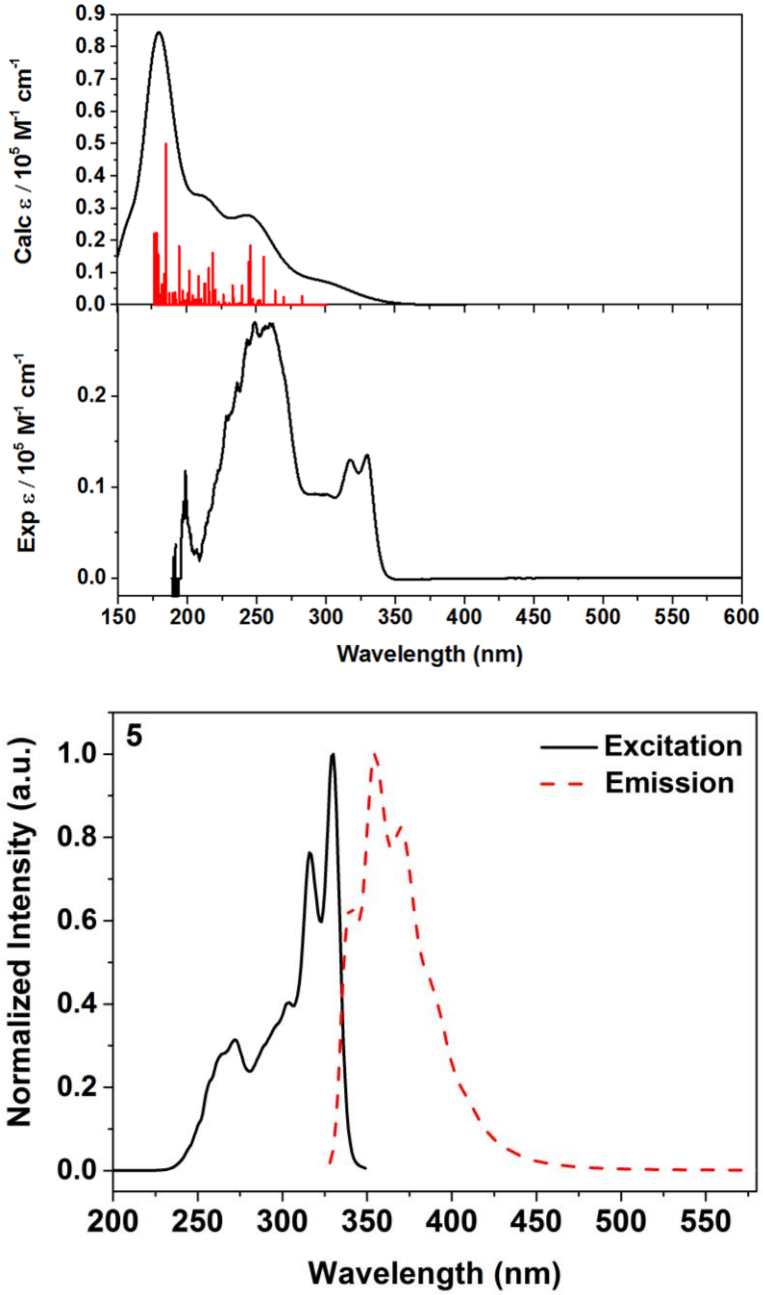


Figure S5. Photophysical spectra for **5** in THF. (top) Experimental and calculated UV-vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line). [**5**] = 0.01 mM.

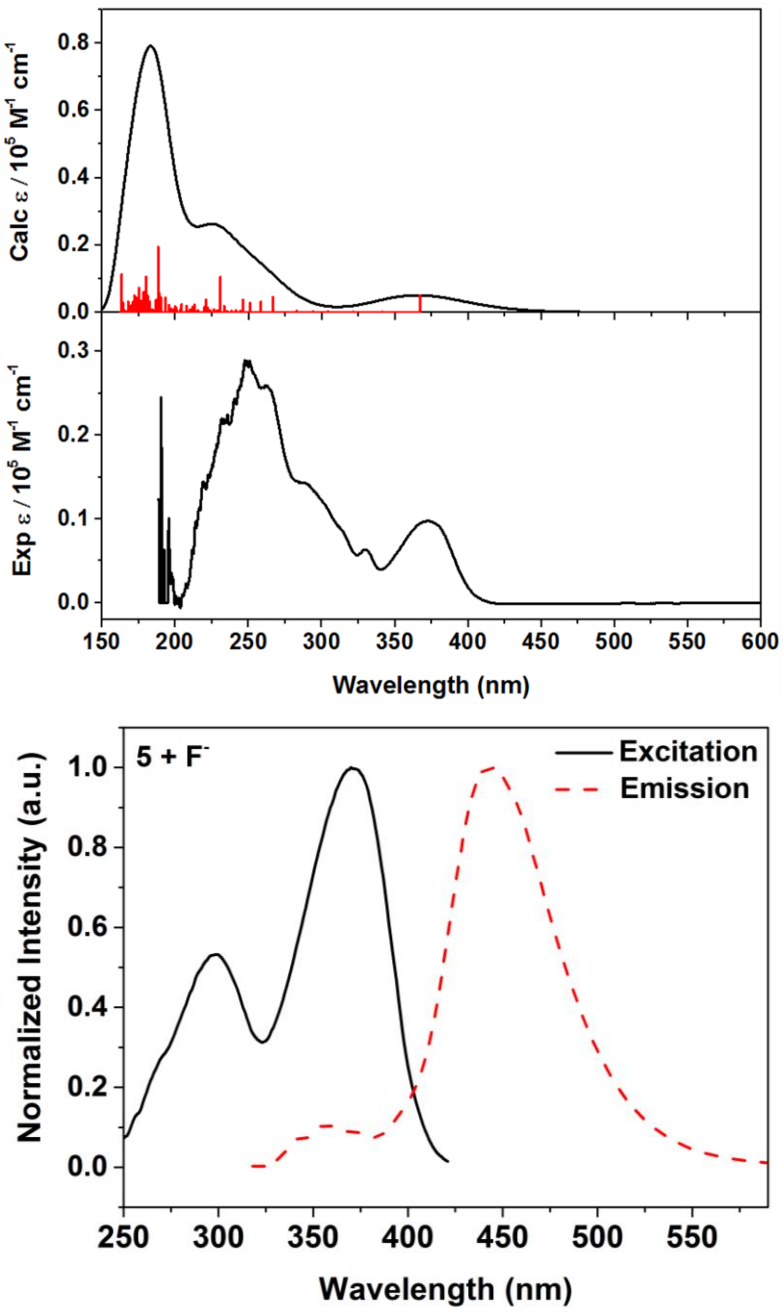


Figure S6. Photophysical spectra for **5** after added F^- in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line).

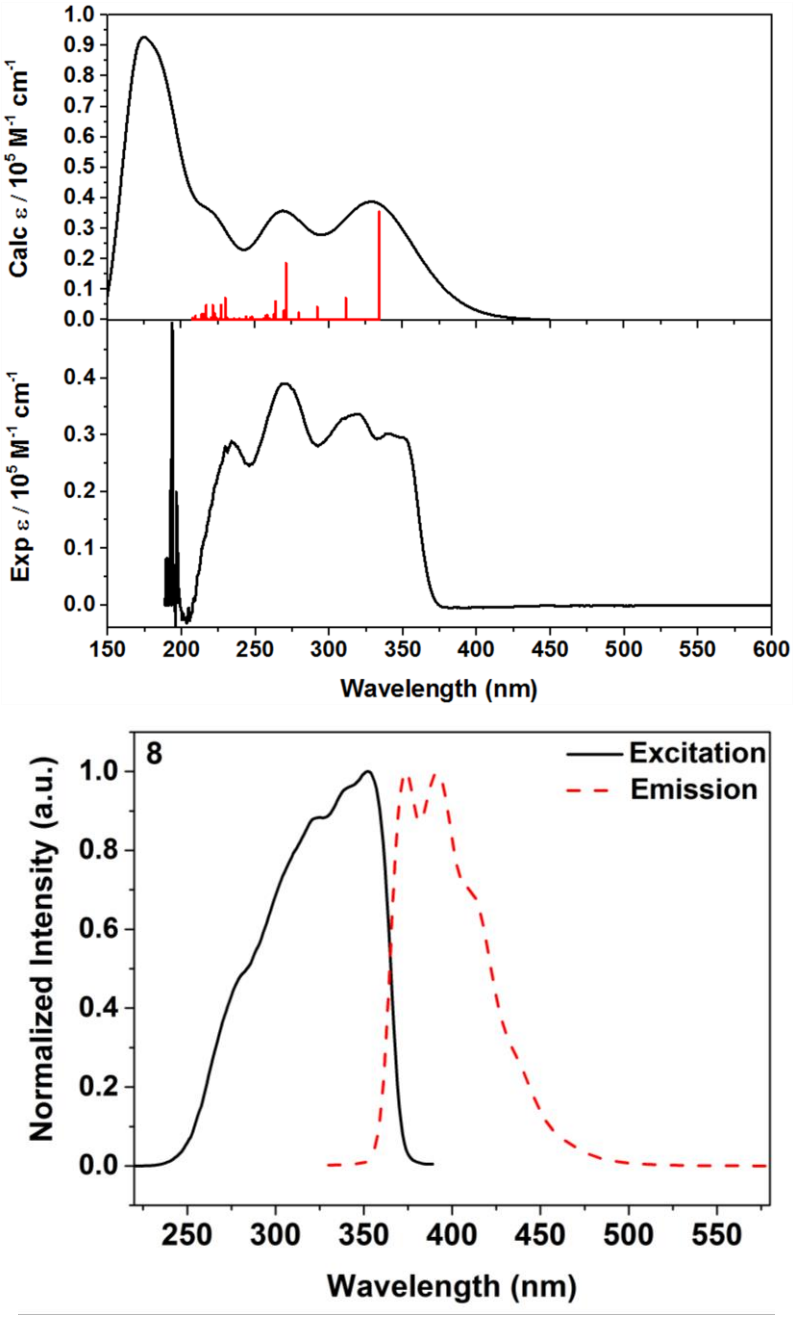


Figure S7. Photophysical spectra for **8** in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line). [**8**] = 0.01 mM.

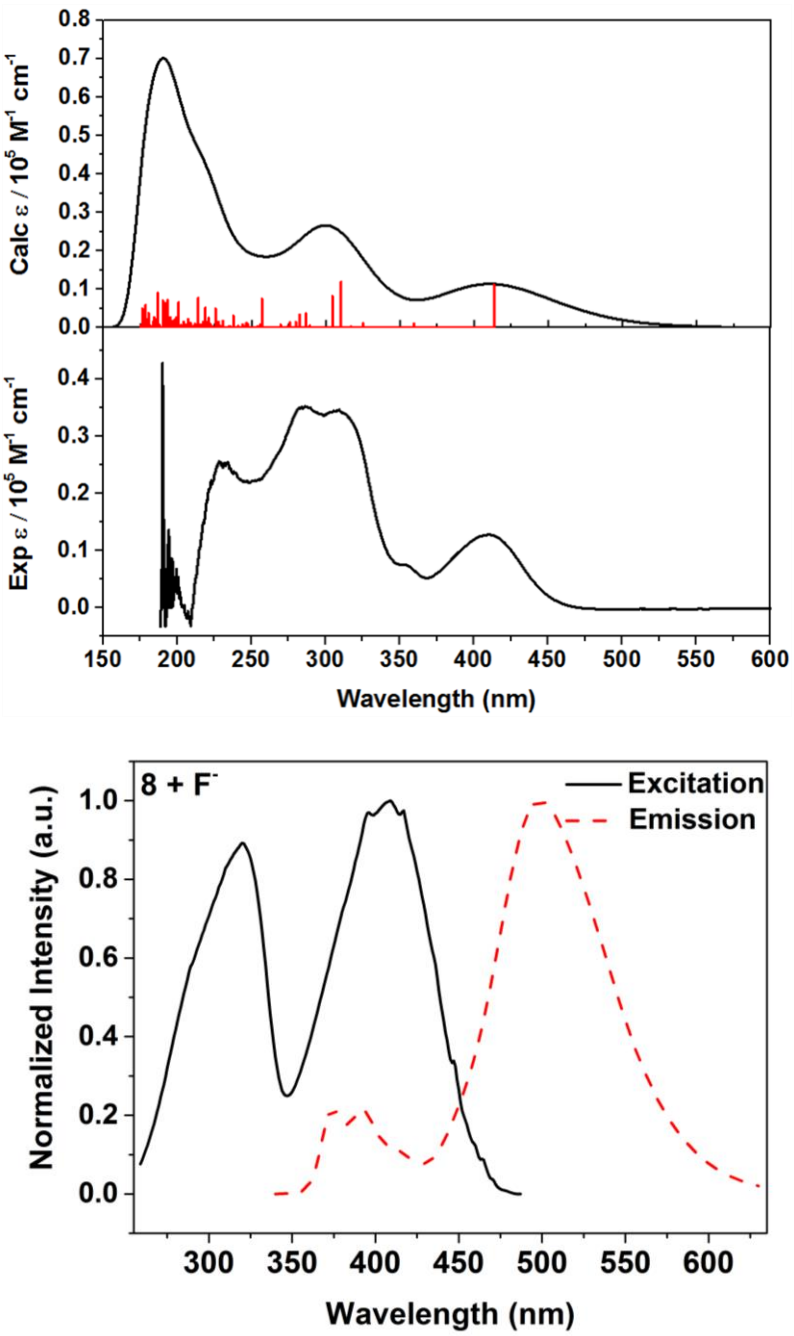


Figure S8. Photophysical spectra for **8** after added F^- in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line).

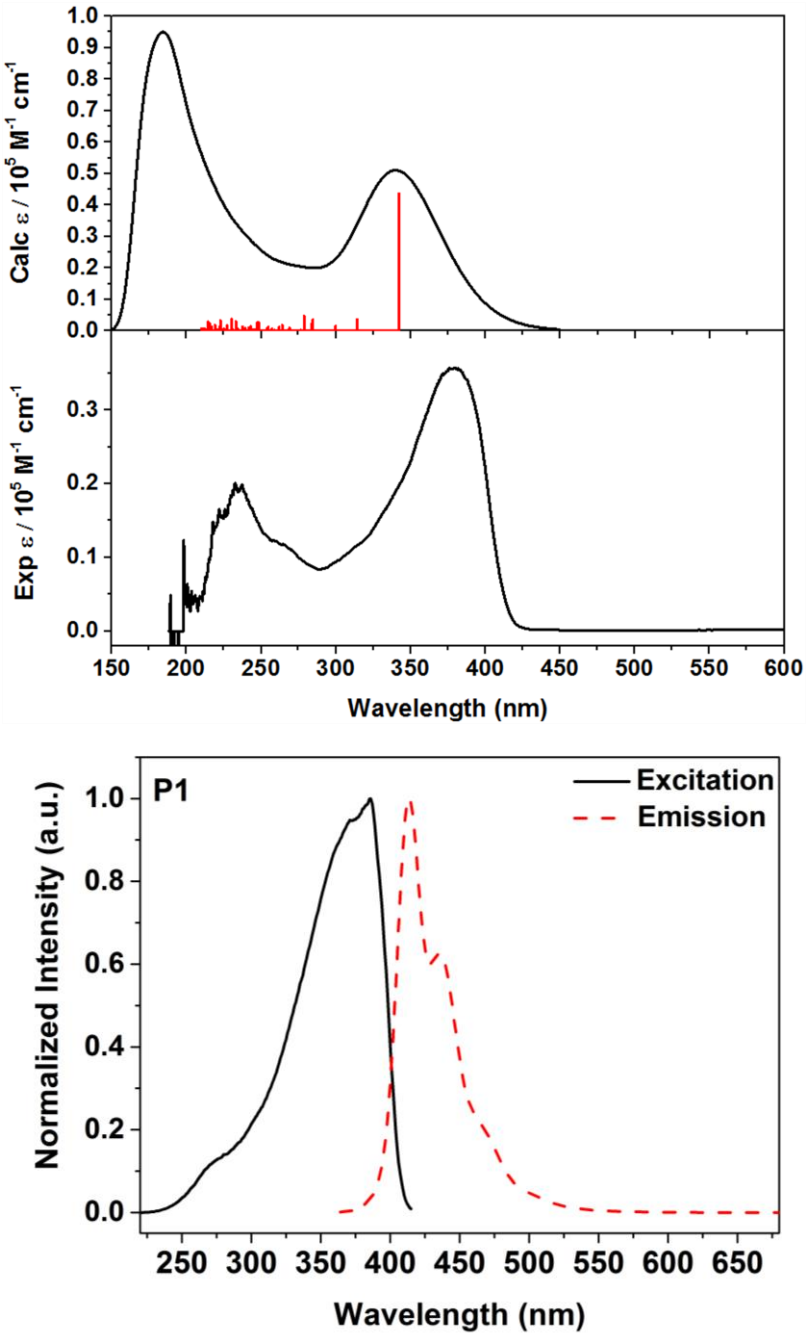


Figure S9. Photophysical spectra for **P1** in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line). [P1] = 0.01 mM.

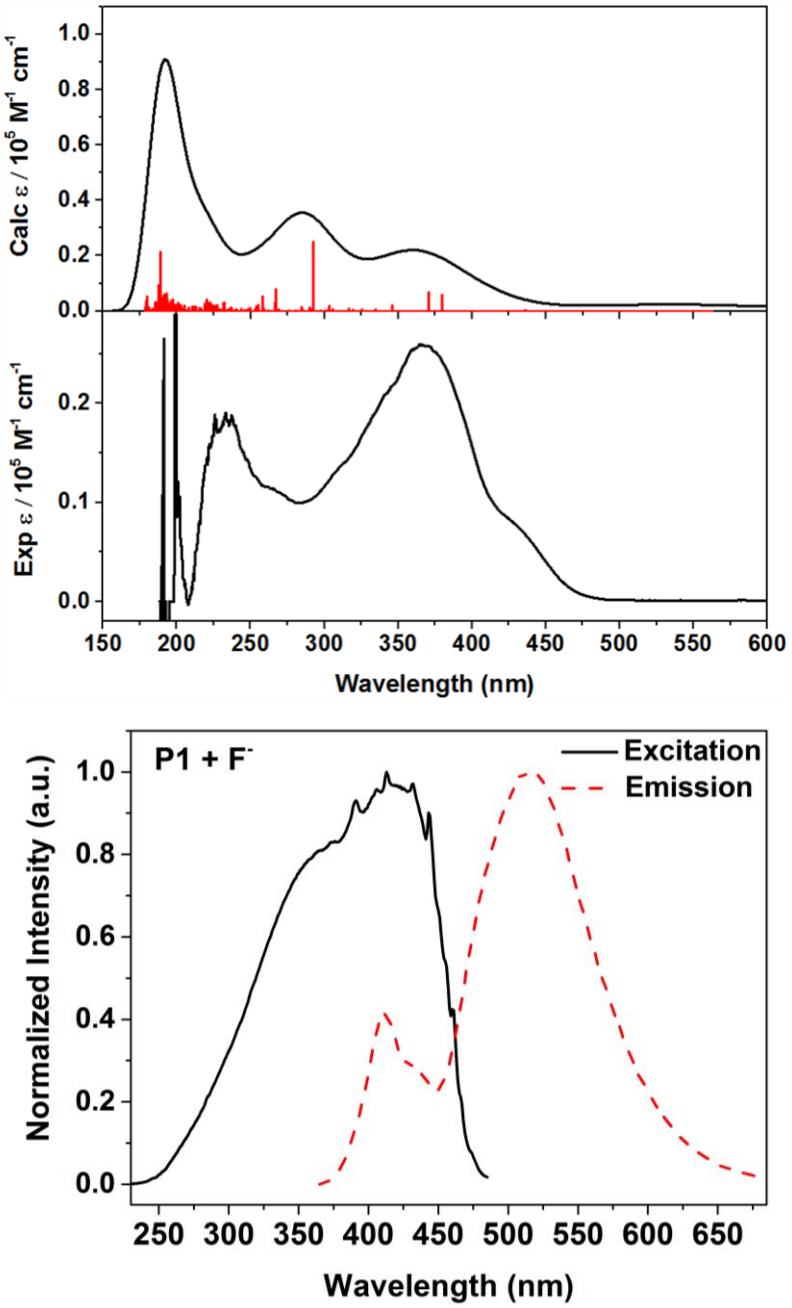


Figure S10. Photophysical spectra for **P1** after added F^- in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line).

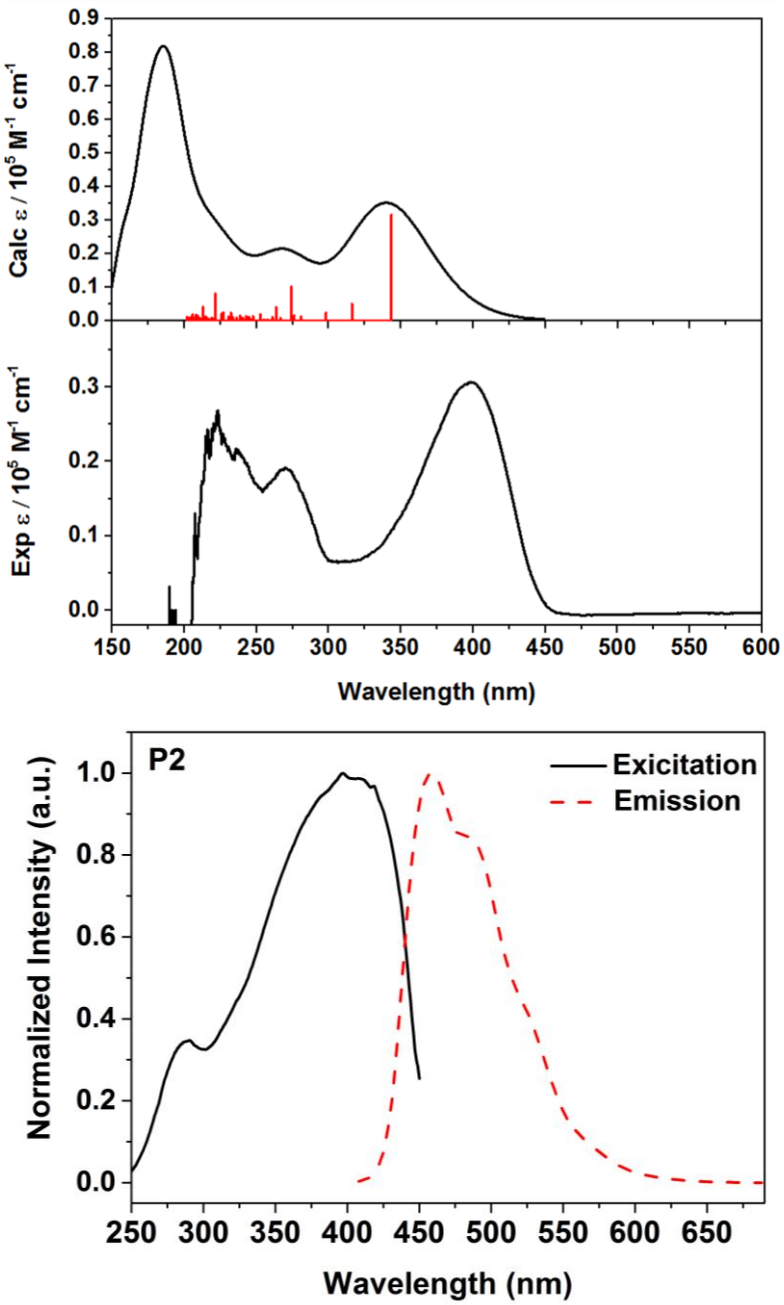


Figure S11. Photophysical spectra for **P2** in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line). [**P2**] = 0.01 mM.

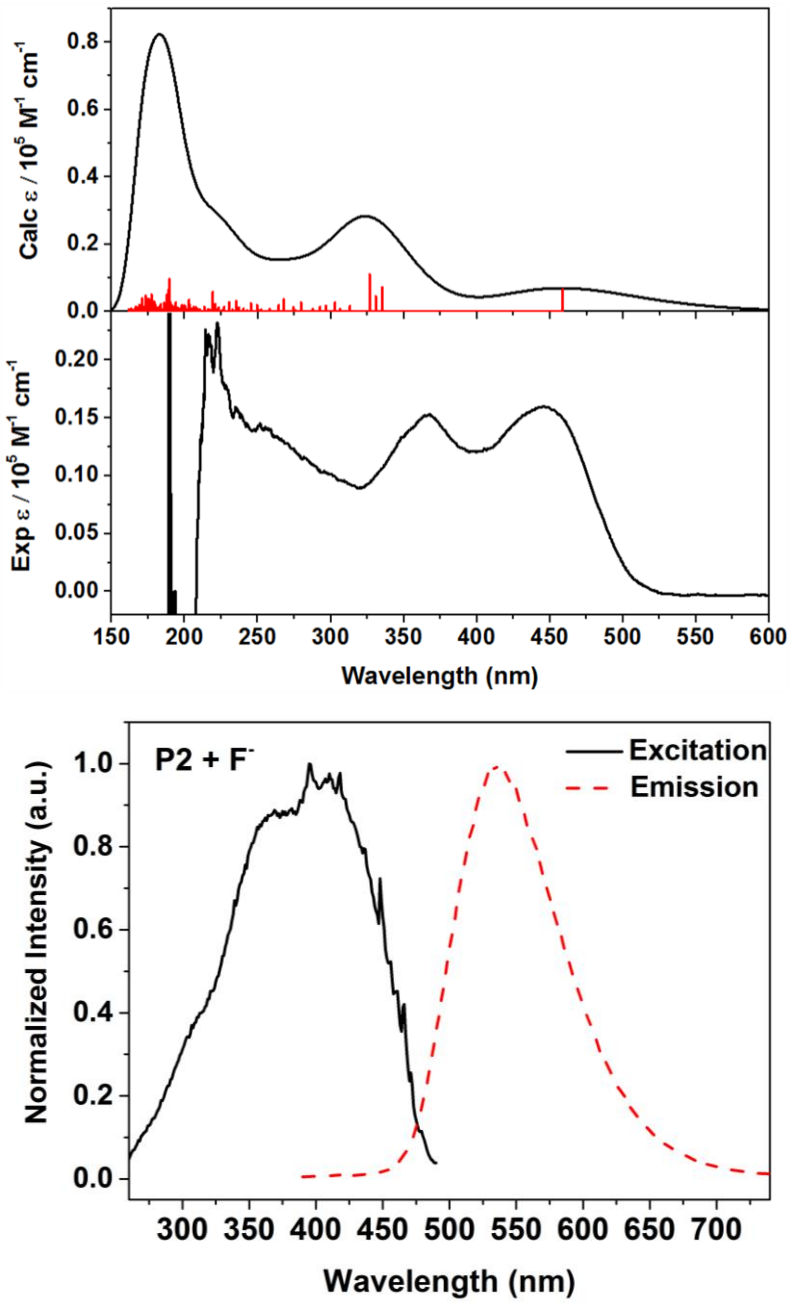


Figure S12. Photophysical spectra for **P1** after added F^- in THF. (top) Experimental and calculated UV/Vis absorbance spectrum; (bottom) Fluorescence excitation (solid line) and emission spectra (dashed line).

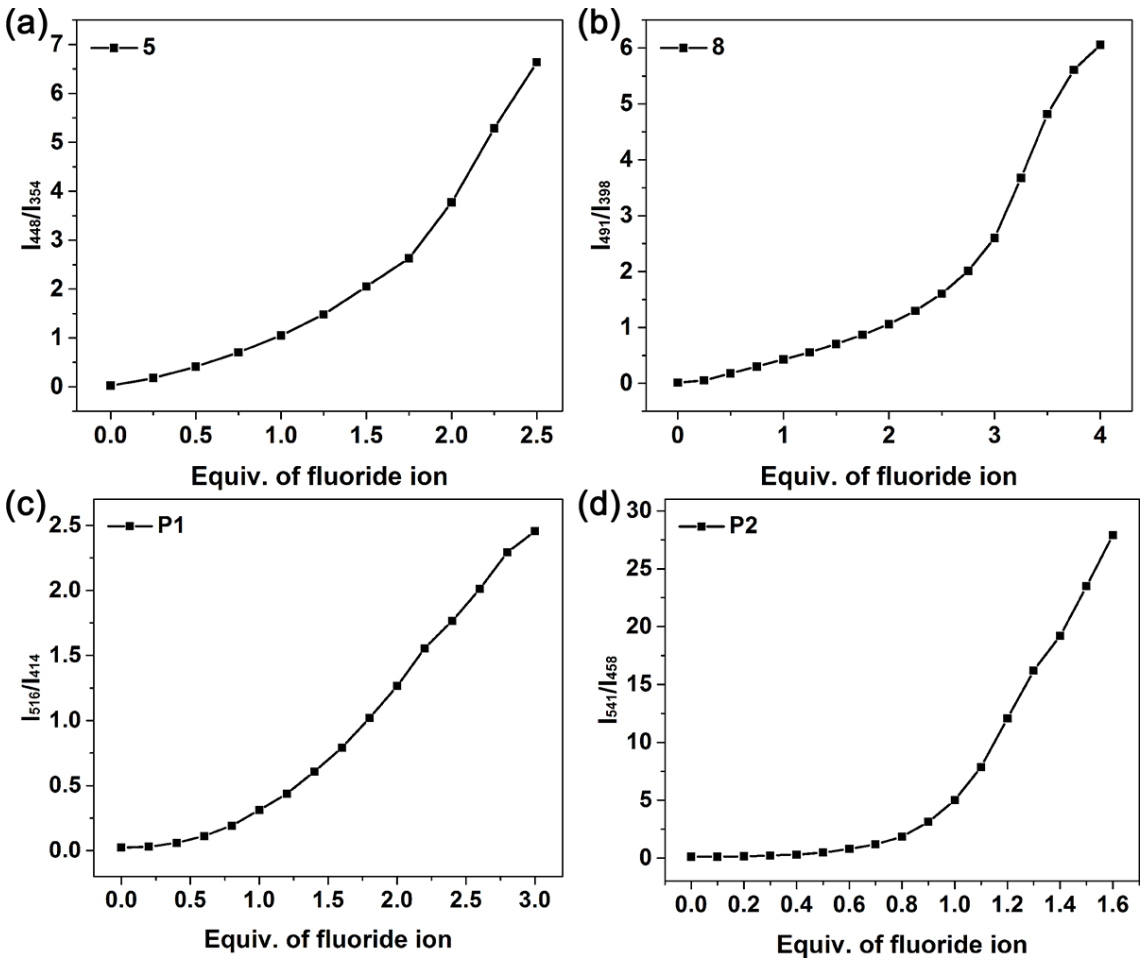


Figure S13. The corresponding ratiometric plot of emission intensity ratio versus equivalents of fluoride. (a) **5**, $\lambda_{em} = I_{448}/I_{354}$; (b) **8**, $\lambda_{em} = I_{498}/I_{391}$; (c) **P1**, $\lambda_{em} = I_{516}/I_{414}$; (d) **P2**, $\lambda_{em} = I_{541}/I_{458}$.

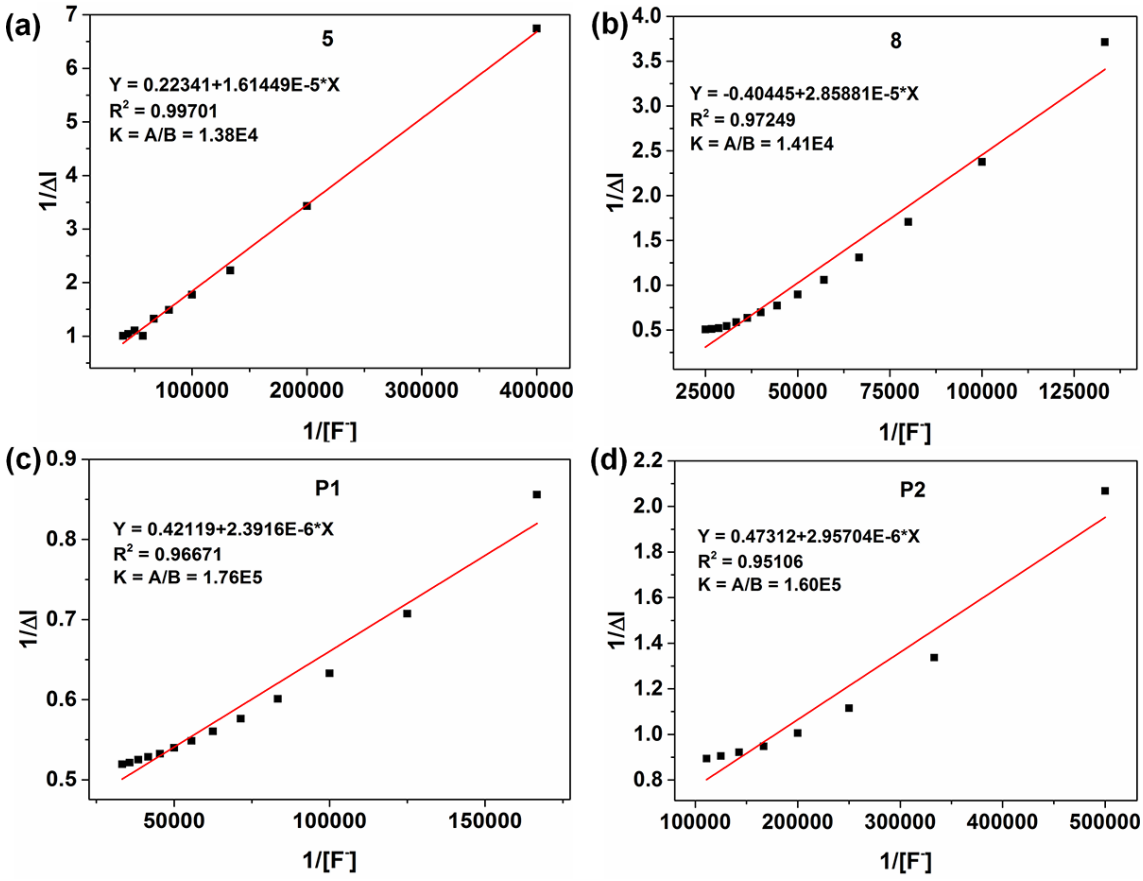


Figure S14. Benesi-Hilderbrand plot of **5** (a), **8** (b), **P1** (c) and **P2** (d) at different [F^-] concentrations. $1/\Delta I = A + B/[F^-]$, $K = A/B$.[28,29]

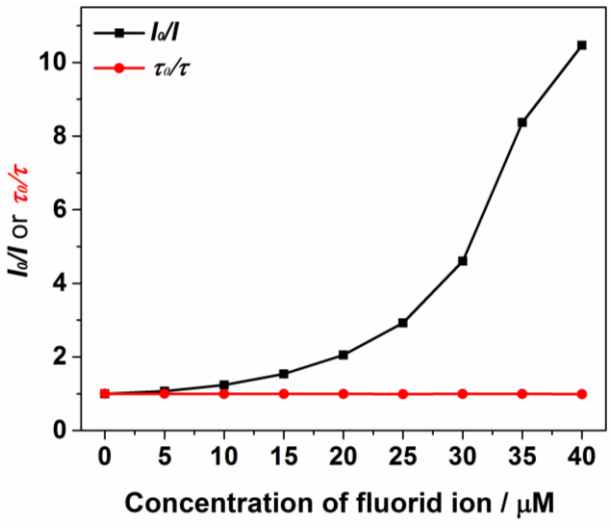


Figure S15. Plots of the ratios of fluorescence intensity (I_0/I) and lifetime change (τ_0/τ) as a function of [F^-] of **8** in THF upon addition of *n*-Bu_4NF, λ_{em} = 391 nm, [**8**] = 10 uM; [F^-] = 1 mM.

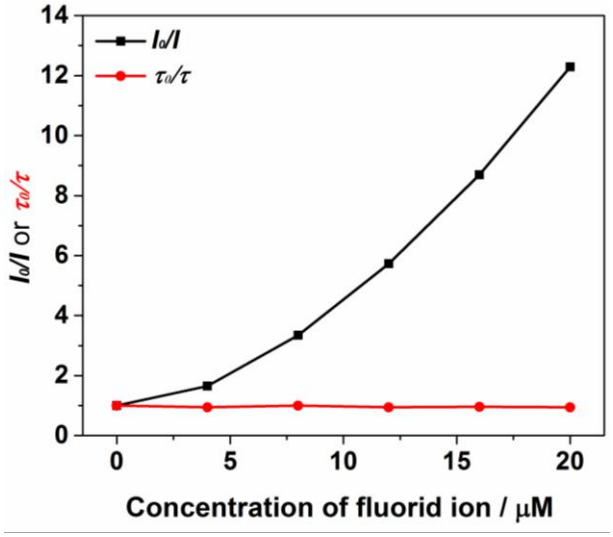


Figure S16. Plots of the ratios of fluorescence intensity (I_0/I) and lifetime change (τ_0/τ) as a function of [F^-] of **P1** in THF upon addition of *n*-Bu_4NF, λ_{em} = 414 nm, [**P1**] = 10 uM; [F^-] = 1 mM.

9. Electrochemical properties

Cyclic voltammograms were recorded with a CHI660E/B15721b electrochemical analyzer using degassed and dried DCM under an argon atmosphere in the glovebox. The CV cell consisted of a gold electrode, a Pt wire counter electrode, and an Ag/AgCl reference electrode. All measurements were performed using DCM solutions of samples with a concentration of 1 mM and 0.1 M $Bu_4N^+PF_6^-$ as a supporting electrolyte with a scan rate of 100 mVs^{-1}. Potentials are determined against a ferrocene/ferrocenyl ion couple (Fc/Fc^+).

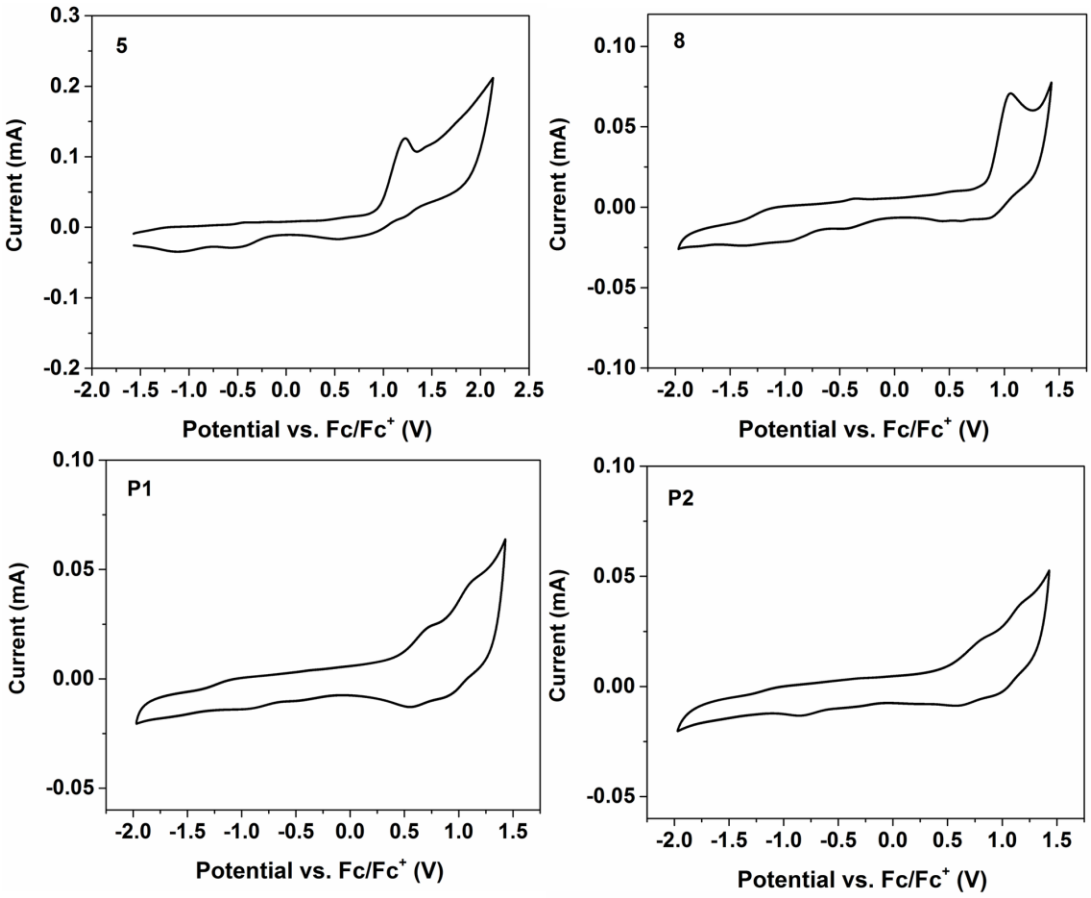


Figure S17. Cyclic voltammograms of **5, 8, P1** and **P2** in DCM with $Bu_4N^+PF_6^-$ (0.1 M) as a supporting electrolyte, Fc = ferrocene.

10. Comparison of HOMO/LUMO plots

Comparison of HOMO/LUMO plots for **5**, **8**, **P1**, **P2**, **5-F**, **5-F'**, **8-F**, **8-F'**, **P1-F**, **P1-F'**, **P2-F**, and **P2-F'** (B3LYP/6-31g*)

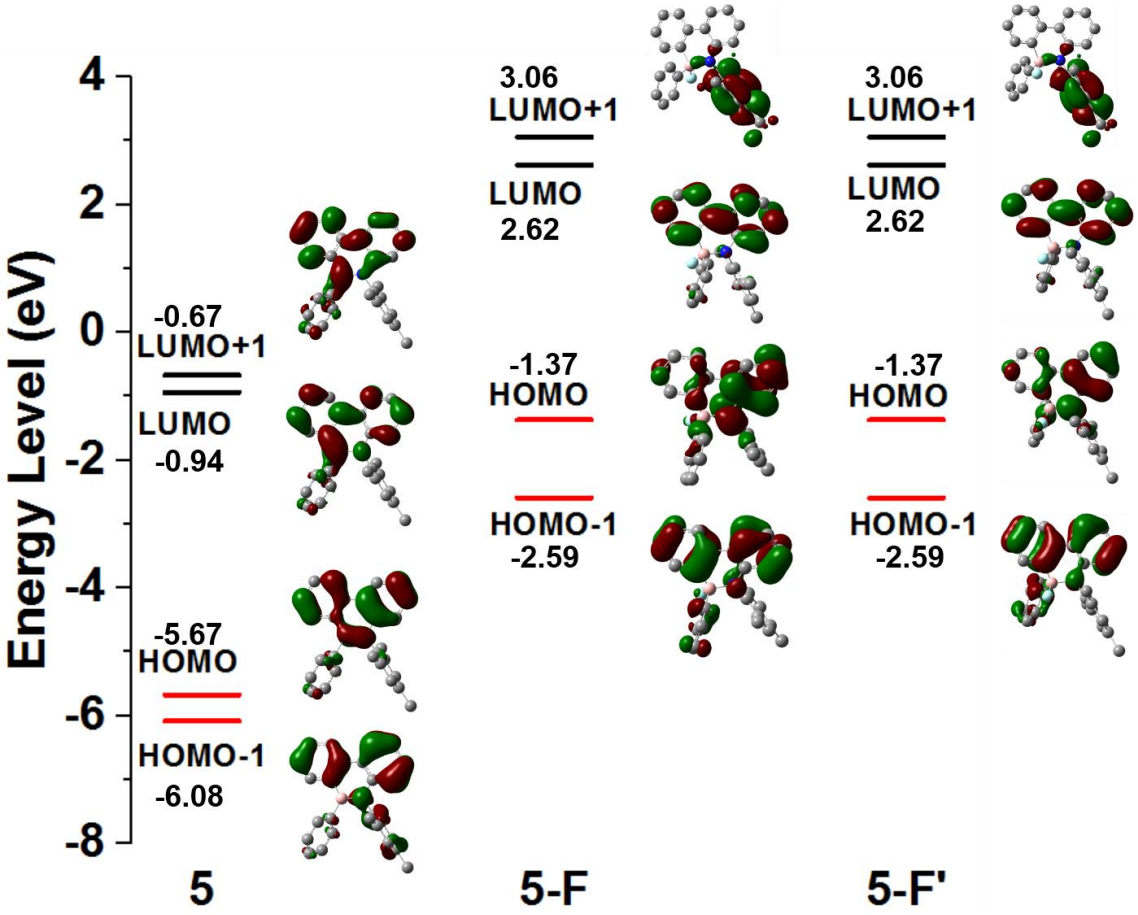


Figure S18. Computed molecular orbital plots for **5** and **5** after added F^- in the gas-phase.

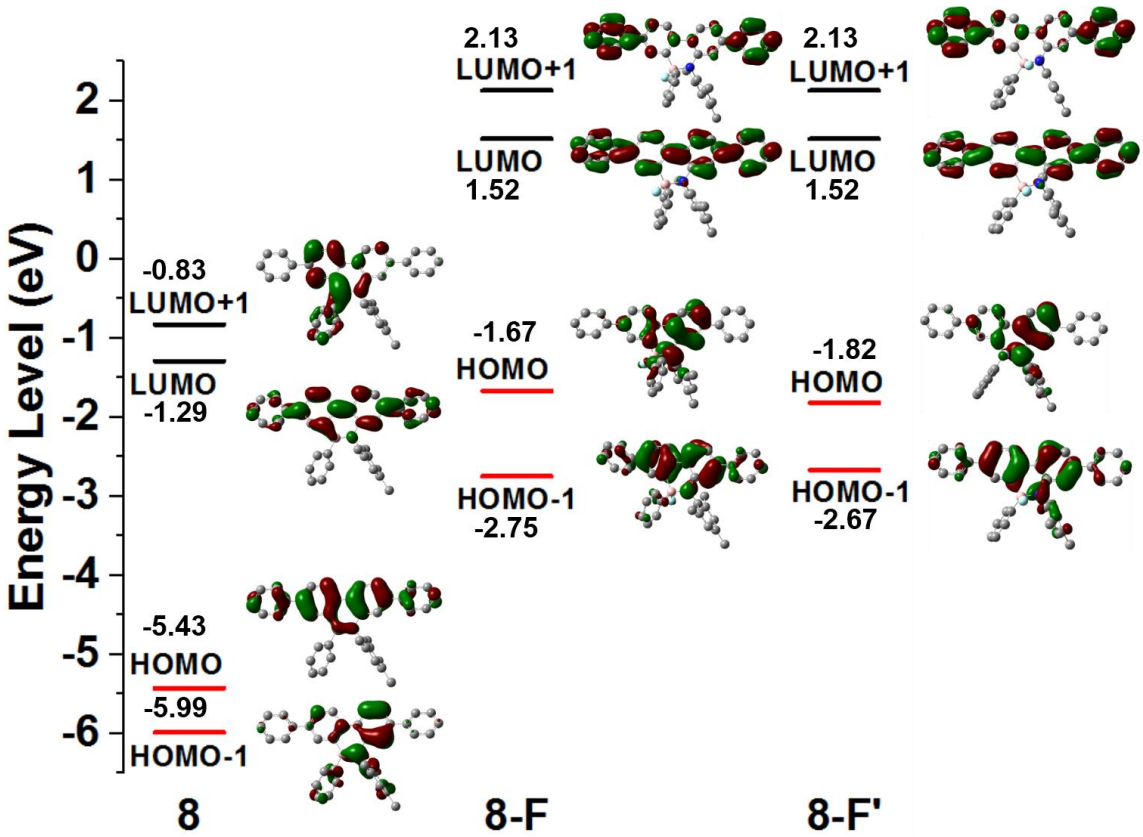


Figure S19. Computed molecular orbital plots for **8** and **8** after added F^- in the gas-phase.

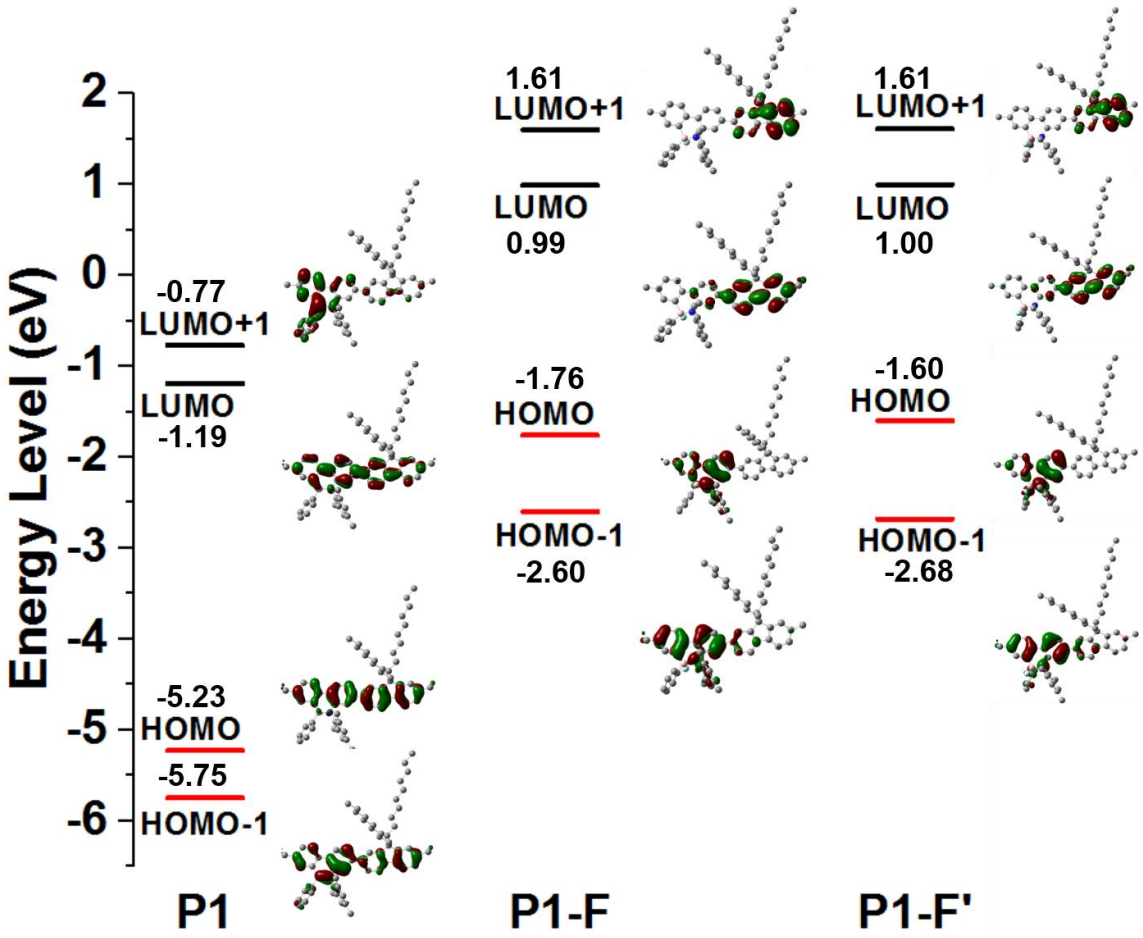


Figure S20. Computed molecular orbital plots for **P1** and after added F^- in the gas-phase.

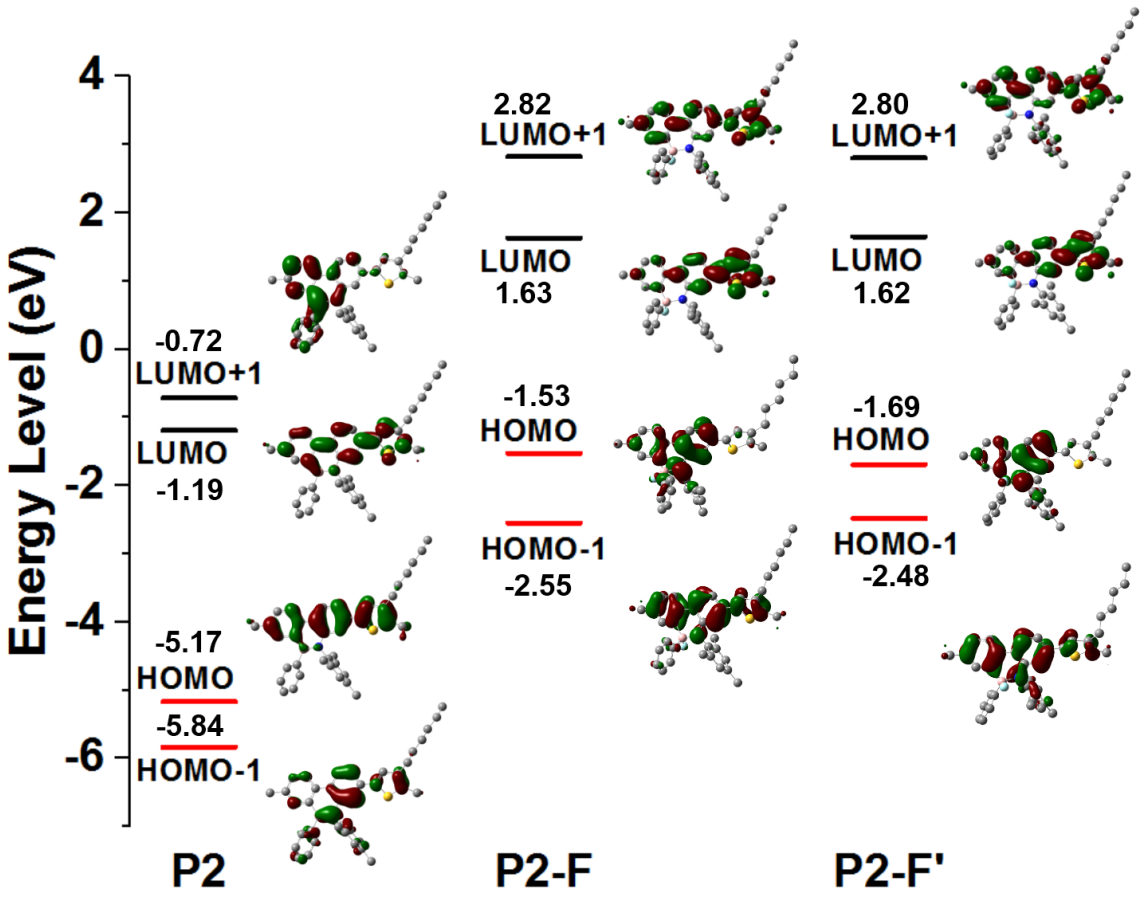


Figure S21. Computed molecular orbital plots for **P2** and after added F^- in the gas-phase.

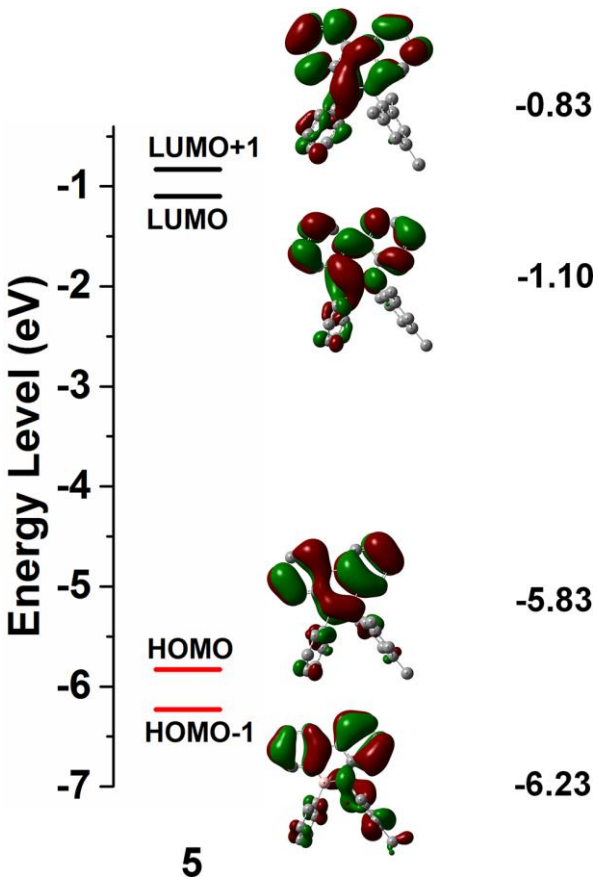


Figure S22. Computed molecular orbital plots for **5** in DCM.

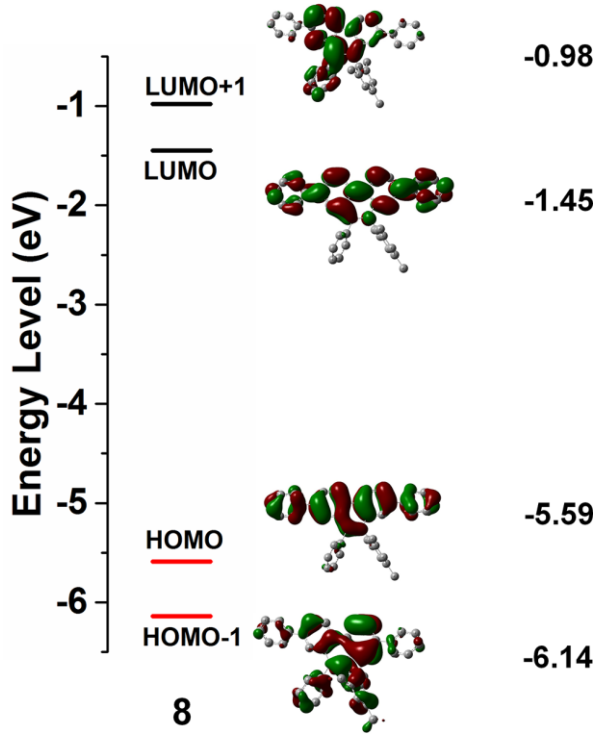


Figure S23. Computed molecular orbital plots for **8** in DCM.

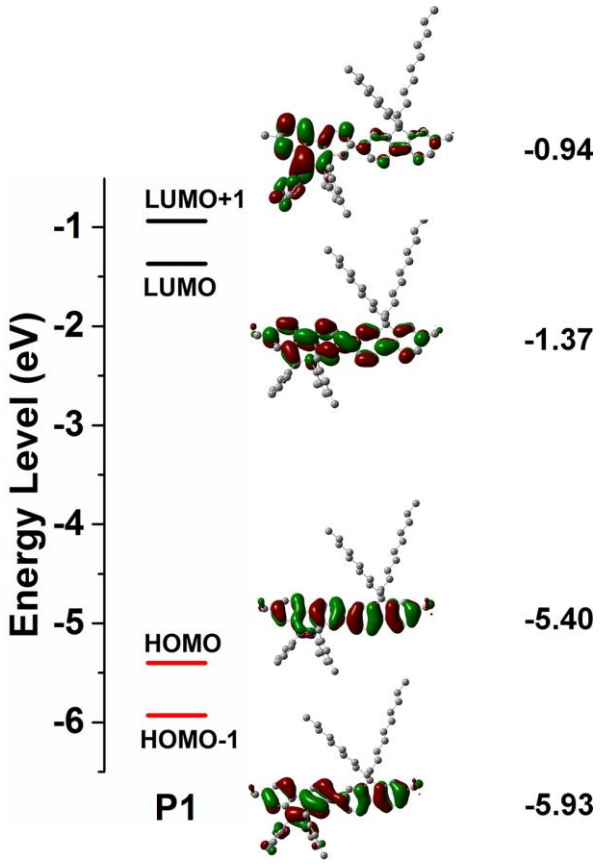


Figure S24. Computed molecular orbital plots for **P1** in DCM.

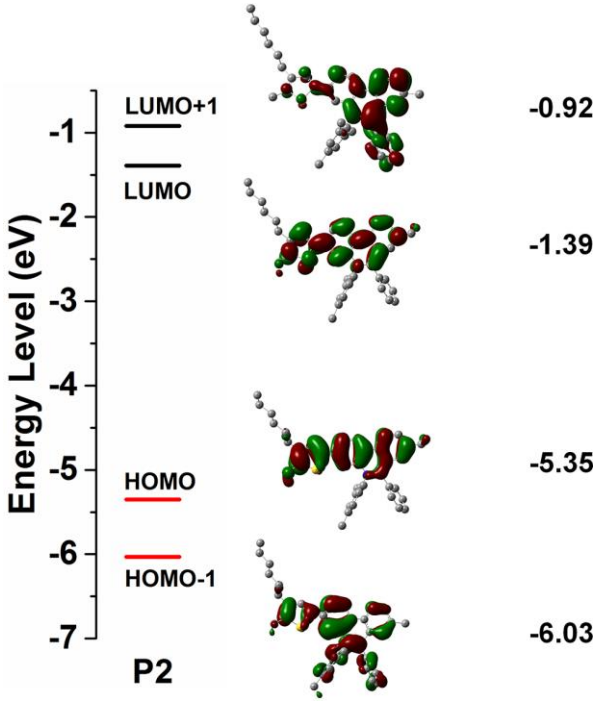


Figure S25. Computed molecular orbital plots for **P2** in DCM.

Table S3. Calculated NICS(0), NICS(0)$_{zz}$, NICS(1) and NICS(1)$_{zz}$, values for **3**, **4**, **5**, **6** and benzene at the b3lyp/6-31g(d) level.

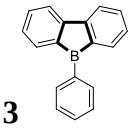
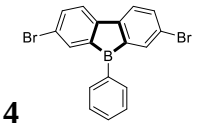
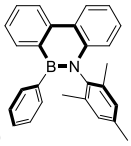
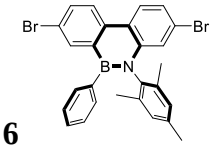
	Benzene	 **3**	 **4**	 **5**	 **6**
NICS(0)	-9.7	+13.8	+12.9	-0.8	-1.0
NICS(0)$_{zz}$	-13.8	+55.0	+53.5	+12.9	+13.1
NICS(1)	-11.2	+6.5	+5.8	-3.7	-3.7
NICS(1)$_{zz}$	-29.0	+26.0	+24.8	-6.9	-6.6

Table S4 Electronic properties of **BNP**-containing small molecules and conjugated polymers.

	HOMO (Exp)[a]	LUMO (Exp)[a]	HOMO (Calc)[b]	LUMO (Calc)[b]	HOMO (Calc)[c]	LUMO (Calc)[c]
5	-5.75	-2.06	-5.83	-1.10	-5.67	-0.94
8	-5.64	-2.25	-5.59	-1.45	-5.43	-1.29
P1	-5.27	-2.23	-5.40	-1.37	-5.23	-1.19
P2	-5.24	-2.39	-5.35	-1.39	5.17	-1.19

[a]Energy levels vs vacuum level were calculated from CV data and from the optically determined energy gap. Theoretical calculations have been carried out by using the GAUSSIAN09 suite of programs in DCM[b] and gas-phase,[c] respectively.

Table S5. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
300.26	0.1388	HOMO-1 ->LUMO+1	12.01%
		HOMO ->LUMO	81.05%
255.32	0.1495	HOMO-4 ->LUMO	47.32%
		HOMO-3 ->LUMO	11.19%
		HOMO-1 ->LUMO+1	23.07%
		HOMO-4 ->LUMO	13.51%
		HOMO-1 ->LUMO+1	24.31%
		HOMO ->LUMO+2	6.92%
		HOMO ->LUMO+3	30.70%
244.32	0.1333	HOMO-6 ->LUMO	5.70%
		HOMO-2 ->LUMO+1	21.82%
		HOMO ->LUMO+3	41.35%

Table S6. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5**-F. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
366.61	0.121	HOMO ->LUMO	96.81%
266.27	0.1099	HOMO-1 ->LUMO	53.85%
		HOMO ->LUMO+5	15.69%
		HOMO ->LUMO+6	21.84%
258.1	0.0758	HOMO-2 ->LUMO	76.48%
		HOMO ->LUMO+6	15.07%
250.64	0.0672	HOMO-3 ->LUMO	37.99%
		HOMO-1 ->LUMO+3	7.62%
		HOMO ->LUMO+6	21.70%
		HOMO ->LUMO+7	7.33%
245.85	0.0898	HOMO-3 ->LUMO	34.03%
		HOMO-1 ->LUMO	13.16%
		HOMO-1 ->LUMO+1	11.43%
		HOMO ->LUMO+6	13.40%
		HOMO ->LUMO+7	14.25%

Table S7. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5**-F'. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
366.61	0.121	HOMO ->LUMO	96.81%
266.27	0.1098	HOMO-1 ->LUMO	53.84%
		HOMO ->LUMO+5	15.70%
		HOMO ->LUMO+6	21.84%
258.1	0.0758	HOMO-2 ->LUMO	76.48%
		HOMO ->LUMO+6	15.07%
250.65	0.0672	HOMO-3 ->LUMO	38.00%
		HOMO-1 ->LUMO+3	7.62%
		HOMO ->LUMO+6	21.70%
		HOMO ->LUMO+7	7.33%
245.85	0.0898	HOMO-3 ->LUMO	34.03%
		HOMO-1 ->LUMO	13.16%
		HOMO-1 ->LUMO+1	11.43%
		HOMO ->LUMO+6	13.40%
		HOMO ->LUMO+7	14.26%
230.35	0.2527	HOMO-1 ->LUMO	5.37%
		HOMO-1 ->LUMO+3	10.48%
		HOMO ->LUMO+6	9.38%
		HOMO ->LUMO+7	41.32%

Table S8. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths (in nm) of **8**. Molecular orbitals (MOs) involved in the main electronic transition， f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
333.85	0.8134	HOMO ->LUMO	88.72%
311.22	0.1639	HOMO-1 ->LUMO	22.56%
		HOMO ->LUMO	6.17%
		HOMO ->LUMO+1	65.58%
291.89	0.0986	HOMO-1 ->LUMO	65.01%
		HOMO ->LUMO+1	19.55%
270.66	0.4262	HOMO-1 ->LUMO+1	76.50%
263.68	0.1387	HOMO-9 ->LUMO	5.78%
		HOMO-6 ->LUMO	7.73%
		HOMO ->LUMO+2	15.11%
		HOMO ->LUMO+3	7.88%
		HOMO ->LUMO+4	29.43%

Table S9. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **8-F**. Molecular orbitals (MOs) involved in the main electronic transition， f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
456.13	0.2833	HOMO ->LUMO	98.54%
324.16	0.618	HOMO-1 ->LUMO	89.60%
303.88	0.1269	HOMO-2 ->LUMO	44.11%
		HOMO ->LUMO+5	23.49%
		HOMO ->LUMO+6	17.09%
291.02	0.0943	HOMO-3 ->LUMO	87.05%
284.93	0.0726	HOMO ->LUMO+8	84.97%
249.65	0.2168	HOMO-7 ->LUMO	28.23%
		HOMO-3 ->LUMO+1	5.91%
		HOMO ->LUMO+10	51.72%

Table S10. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **8-F'**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
430.22	0.2799	HOMO ->LUMO	98.06%
328.76	0.7238	HOMO-1 ->LUMO	89.46%
250.75	0.2169	HOMO-7 ->LUMO	11.56%
		HOMO ->LUMO+10	61.70%

Table S11. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **P1**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
342.24	1.1913	HOMO -> LUMO	95.51%
313.82	0.0994	HOMO-2 -> LUMO	6.22%
		HOMO-1 -> LUMO	21.72%
		HOMO -> LUMO+1	60.56%
284.43	0.0977	HOMO-8 -> LUMO	8.01%
		HOMO-1 -> LUMO+1	13.30%
		HOMO -> LUMO+2	50.39%
		HOMO -> LUMO+3	12.79%
278.58	0.1306	HOMO-8 -> LUMO	9.34%
		HOMO-1 -> LUMO+1	19.58%
		HOMO -> LUMO+3	43.73%
230.31	0.102	HOMO-10 -> LUMO	32.70%
		HOMO-9 -> LUMO+1	10.11%
		HOMO-6 -> LUMO+1	12.86%
		HOMO-1 -> LUMO+6	13.72%

Table S12. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths (in nm) of **P1-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
523.68	0.0848	HOMO -> LUMO	99.15%
385.26	0.4947	HOMO-1 -> LUMO	96.20%
357.25	0.0996	HOMO -> LUMO+2	93.60%
350.05	0.1597	HOMO -> LUMO+3	93.47%
292.68	0.5243	HOMO-6 -> LUMO	81.37%
		HOMO-1 -> LUMO+3	7.54%
269.02	0.0774	HOMO-1 -> LUMO+3	13.12%
		HOMO -> LUMO+6	5.28%
		HOMO -> LUMO+7	15.81%
		HOMO -> LUMO+10	53.50%

Table S13. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **P1-F'**. Molecular orbitals (MOs) involved in the main electronic transition, f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*).

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
562.01	0.0853	HOMO -> LUMO	99.28%
379.28	0.1152	HOMO-1 -> LUMO	49.07%
		HOMO -> LUMO+2	33.01%
		HOMO -> LUMO+3	13.15%
374.06	0.4199	HOMO-1 -> LUMO	43.65%
		HOMO -> LUMO+2	53.38%
370.37	0.1344	HOMO-1 -> LUMO	5.59%
		HOMO -> LUMO+2	9.19%
		HOMO -> LUMO+3	81.61%
292.36	0.498	HOMO-7 -> LUMO	79.80%
		HOMO -> LUMO+8	10.06%
266.74	0.1547	HOMO-1 -> LUMO+3	20.00%
		HOMO -> LUMO+10	21.14%
		HOMO -> LUMO+11	15.77%
		HOMO -> LUMO+13	18.65%
266.2	0.0549	HOMO-2 -> LUMO+2	34.99%
		HOMO-2 -> LUMO+3	44.44%
		HOMO -> LUMO+13	6.06%

257.79	0.1041	HOMO-9 -> LUMO	11.57%
		HOMO-5 -> LUMO+1	9.55%
		HOMO -> LUMO+13	38.39%

Table S14. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **P2**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
343.24	0.7838	HOMO ->LUMO	91.13%
315.8	0.1213	HOMO-1 ->LUMO	21.43%
		HOMO ->LUMO	6.01%
		HOMO ->LUMO+1	66.01%
273.95	0.2484	HOMO-2 ->LUMO	10.41%
		HOMO-1 ->LUMO+1	53.19%
		HOMO ->LUMO+3	17.45%
263.47	0.0973	HOMO-6 ->LUMO	27.31%
		HOMO-3 ->LUMO	11.04%
		HOMO-2 ->LUMO+1	7.98%
		HOMO ->LUMO+2	10.47%
		HOMO ->LUMO+3	9.86%
		HOMO ->LUMO+4	13.79%

Table S15. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths (in nm) of **P2-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
458.37	0.1703	HOMO ->LUMO	98.20%
334.93	0.1853	HOMO-1 ->LUMO	50.82%
		HOMO ->LUMO+1	43.58%
330.48	0.1168	HOMO-1 ->LUMO	18.61%
		HOMO ->LUMO+1	12.17%
		HOMO ->LUMO+2	65.98%
326.27	0.2849	HOMO-1 ->LUMO	23.58%
		HOMO ->LUMO+1	38.71%
		HOMO ->LUMO+2	25.71%
		HOMO ->LUMO+3	6.25%

267.5	0.0915	HOMO-8 ->LUMO	10.38%
		HOMO-7 ->LUMO	57.41%
		HOMO-1 ->LUMO+1	9.12%
		HOMO ->LUMO+8	13.15%

Table S16. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths (in nm) of **P2-F'**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-DFT, B3LYP/6-31g*)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
431.81	0.1618	HOMO ->LUMO	97.37%
337.15	0.4565	HOMO-1 ->LUMO	88.78%
		HOMO ->LUMO+1	6.15%
318.12	0.1694	HOMO ->LUMO+1	75.32%
		HOMO ->LUMO+2	16.89%
313.58	0.0756	HOMO ->LUMO+1	9.65%
		HOMO ->LUMO+2	60.04%
		HOMO ->LUMO+3	24.87%
307.57	0.099	HOMO ->LUMO+1	5.16%
		HOMO ->LUMO+2	16.99%
		HOMO ->LUMO+3	71.06%
262.14	0.108	HOMO-7 ->LUMO	17.71%
		HOMO-1 ->LUMO+1	10.64%
		HOMO ->LUMO+7	9.81%
		HOMO ->LUMO+8	50.19%
250.1	0.0968	HOMO-7 ->LUMO	13.57%
		HOMO-1 ->LUMO+1	27.82%
		HOMO-1 ->LUMO+2	9.51%
		HOMO-1 ->LUMO+3	11.54%
		HOMO ->LUMO+8	14.08%

11. ^{1}H NMR and ^{13}C NMR spectra

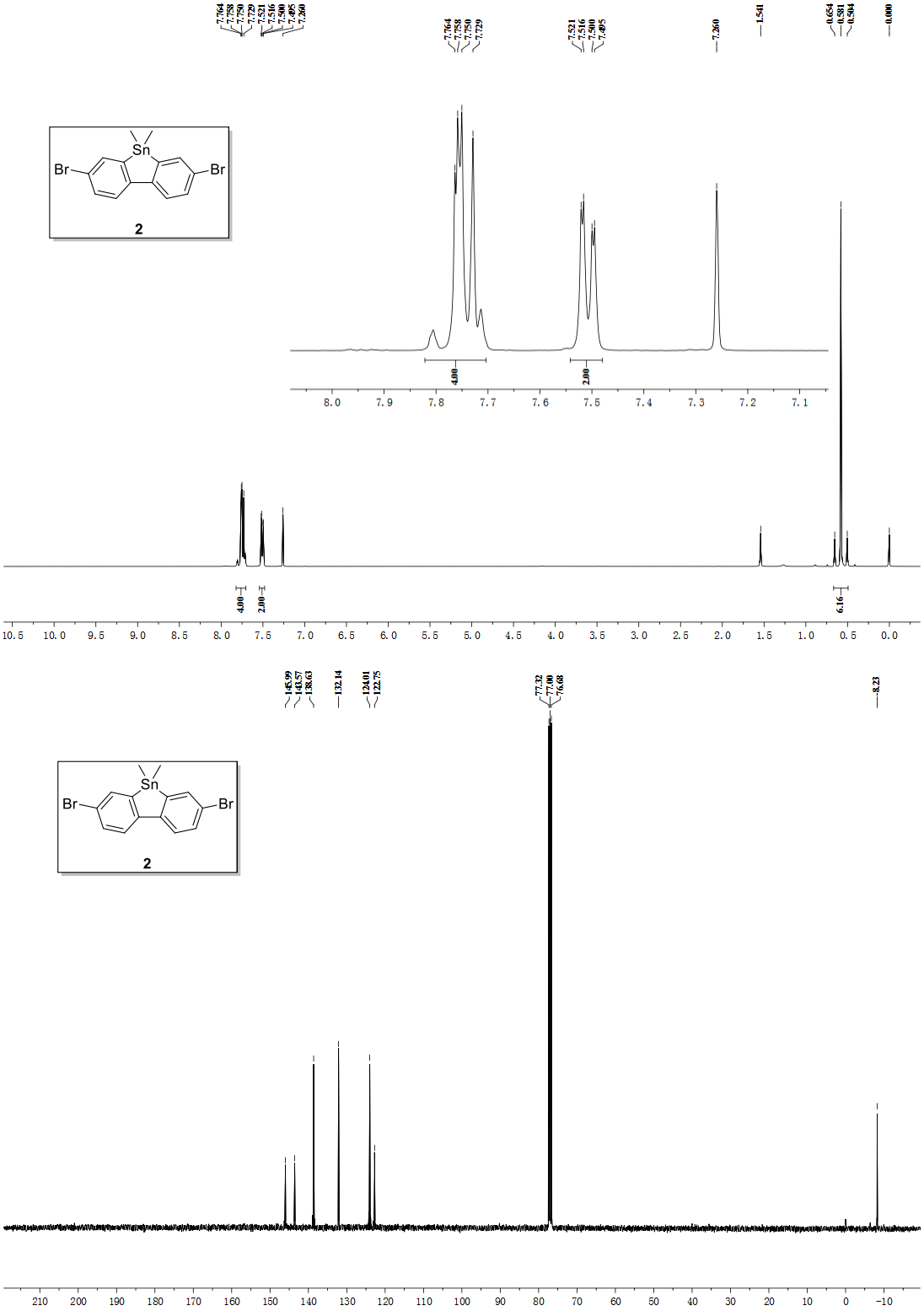


Figure S26. ^{1}H and ^{13}C NMR spectra of **2** in $CDCl_3$.

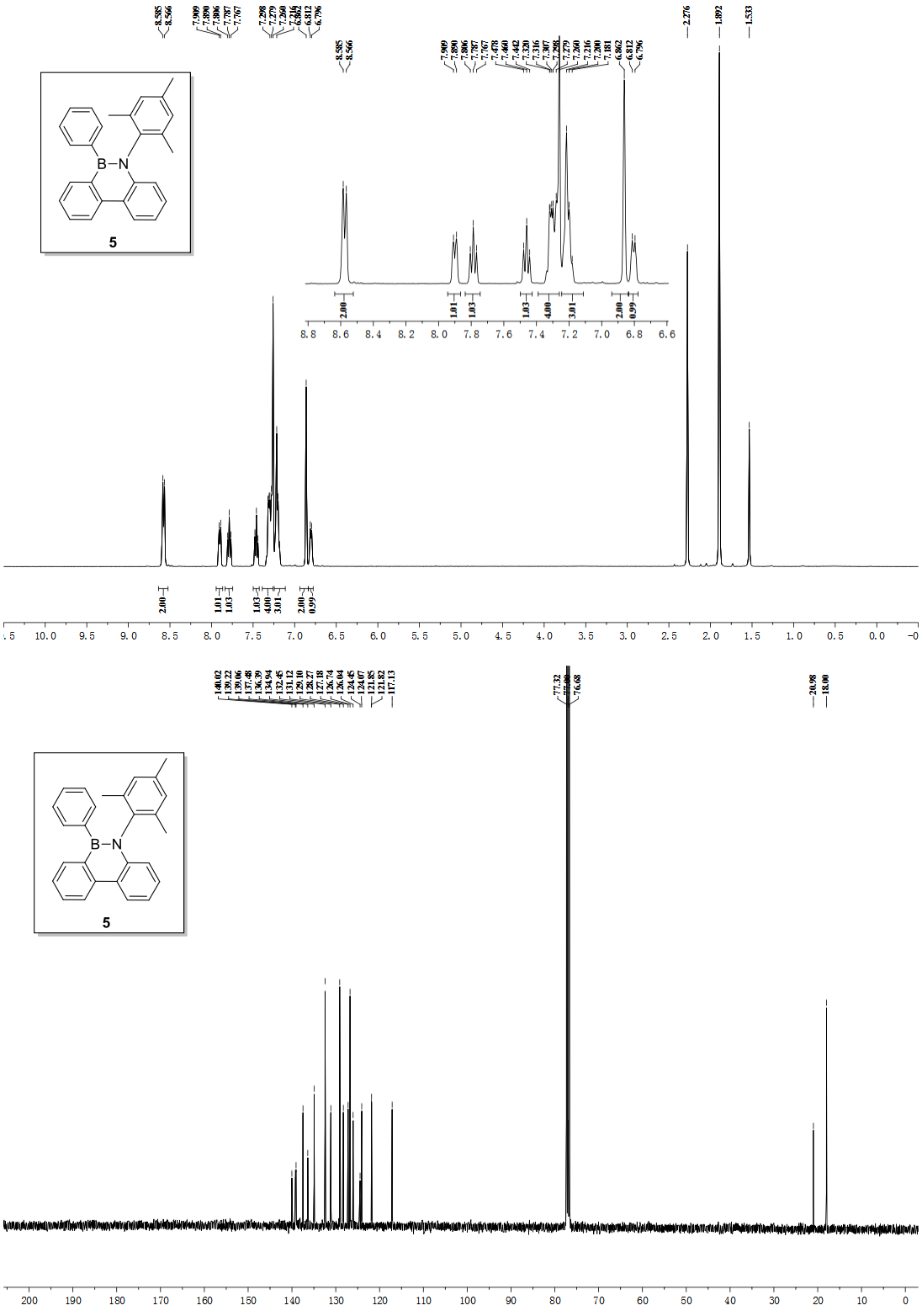


Figure S27. ^{1}H and ^{13}C NMR spectra of **5** in $CDCl_3$.

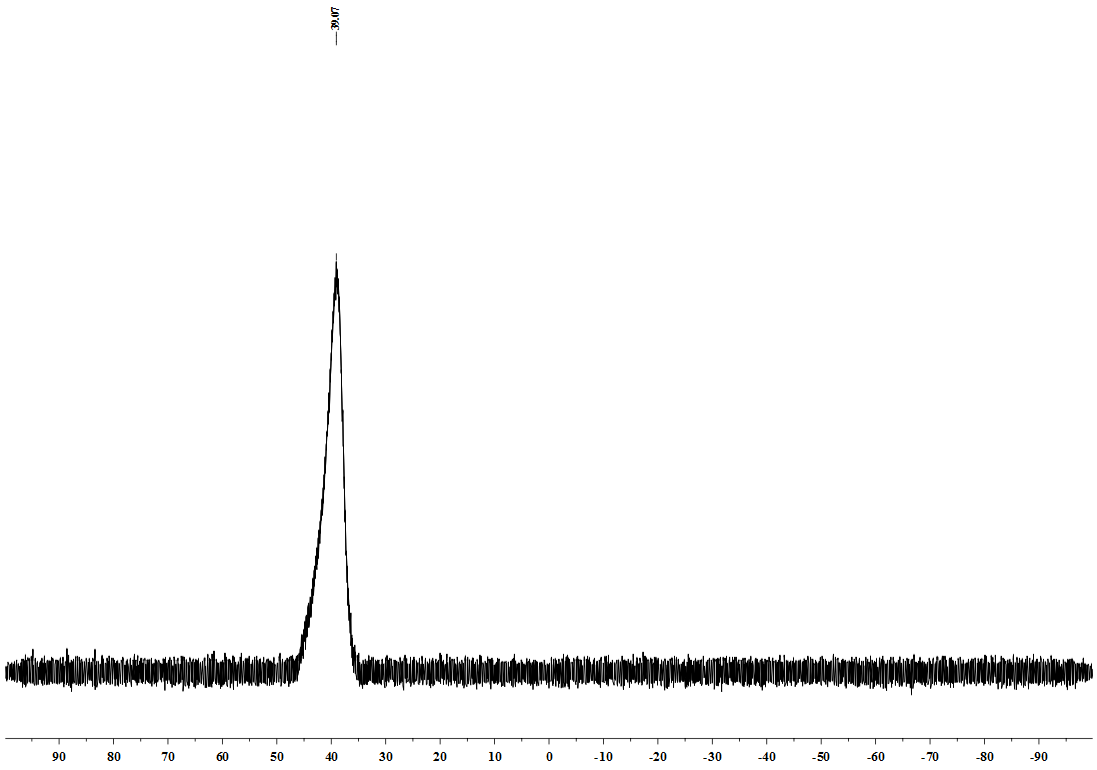


Figure S28. ^{11}B NMR spectra of **5** in $CDCl_3$**.**

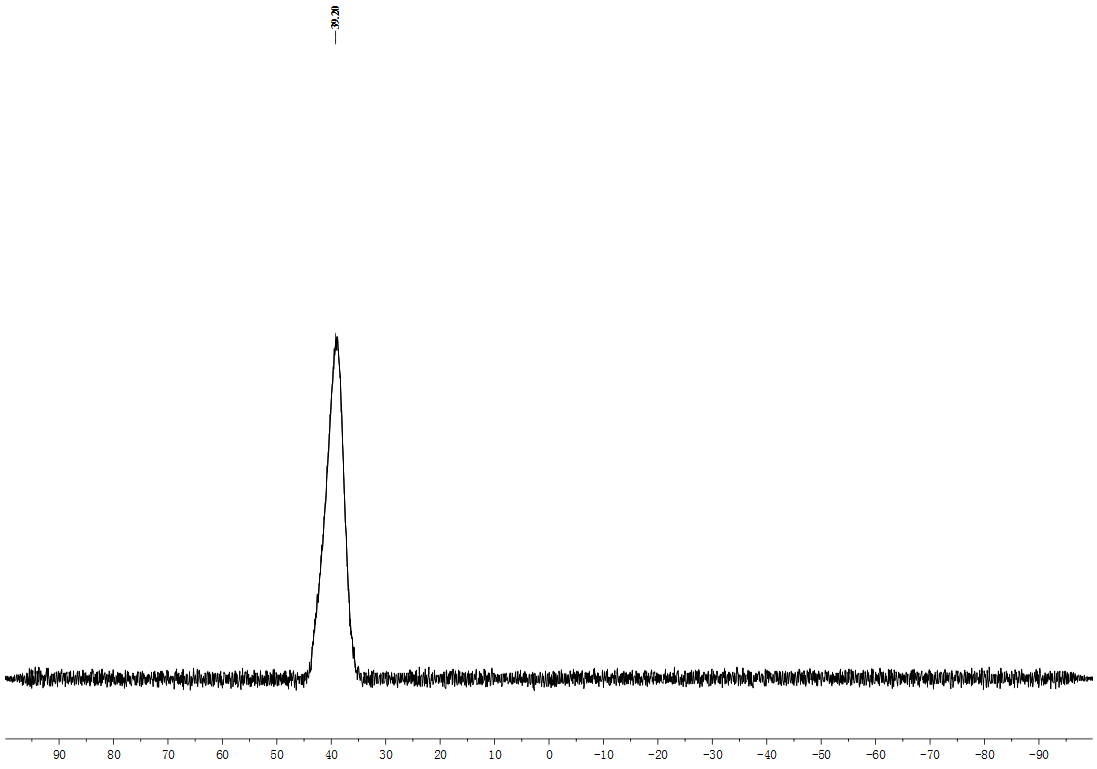


Figure S29. ^{11}B NMR spectra of **6** in $CDCl_3$**.**

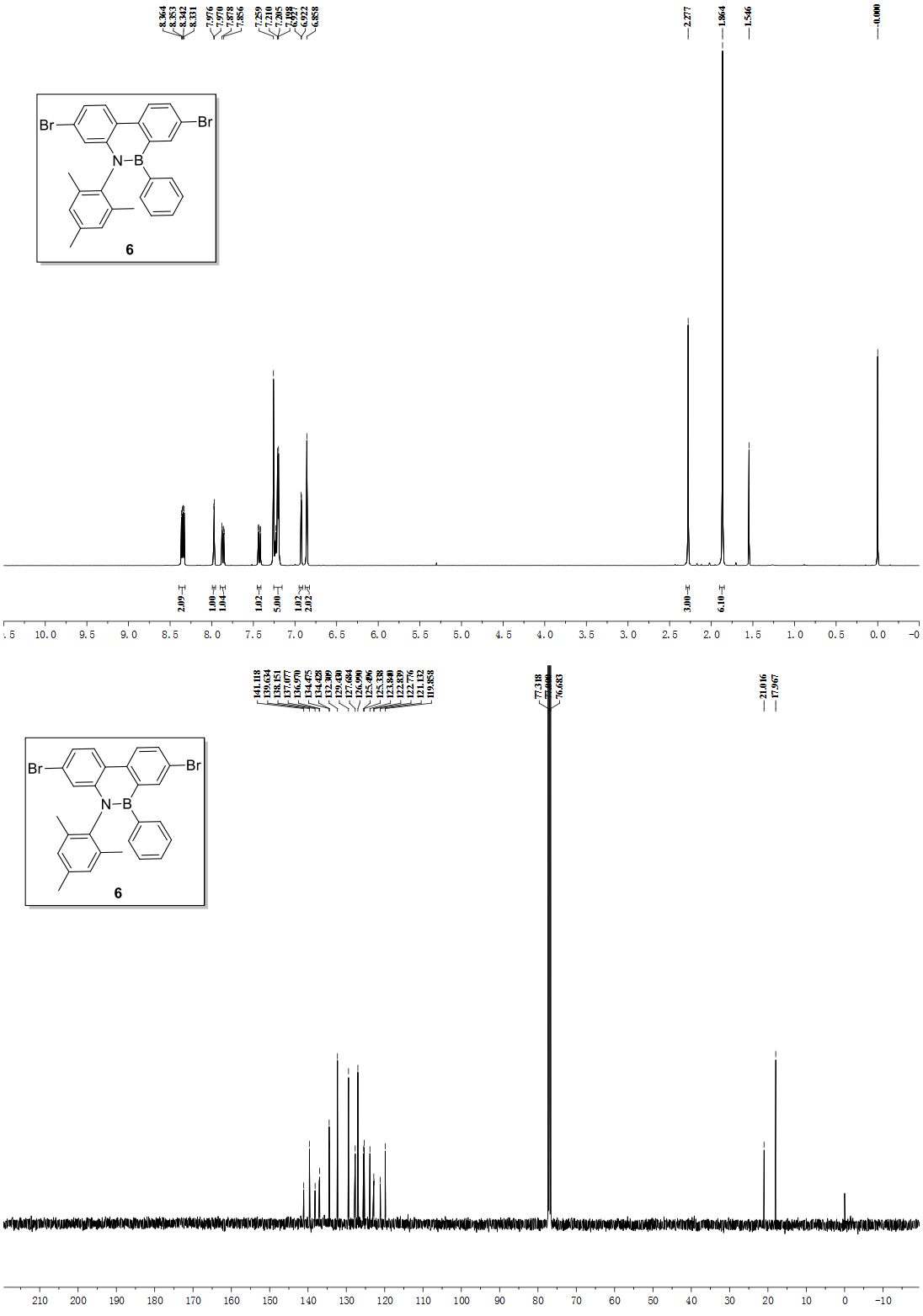


Figure S30. ^{1}H and ^{13}C NMR spectra of **6** in $CDCl_3$.

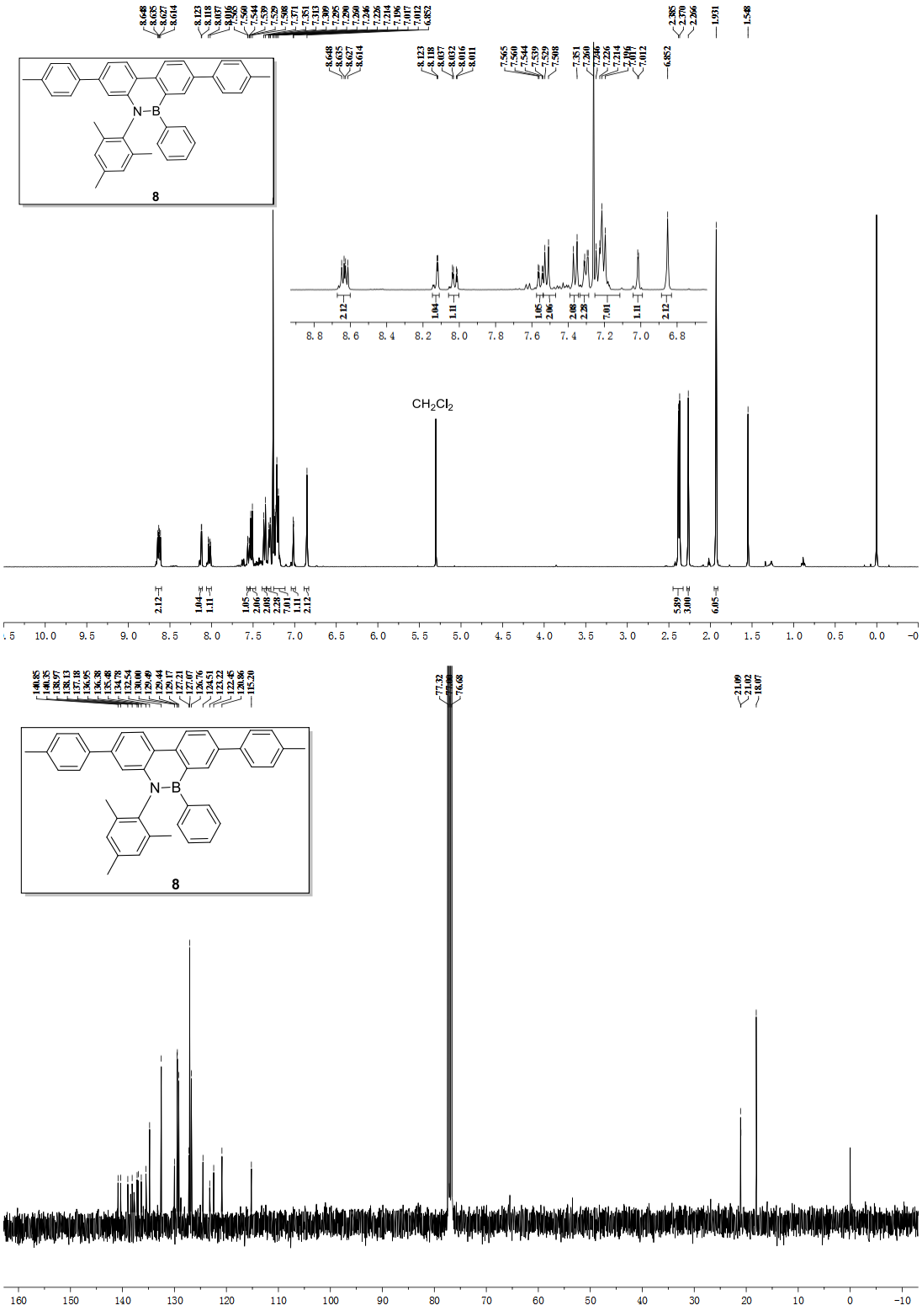


Figure S31. ^{1}H and ^{13}C NMR spectra of **8** in $CDCl_3$.

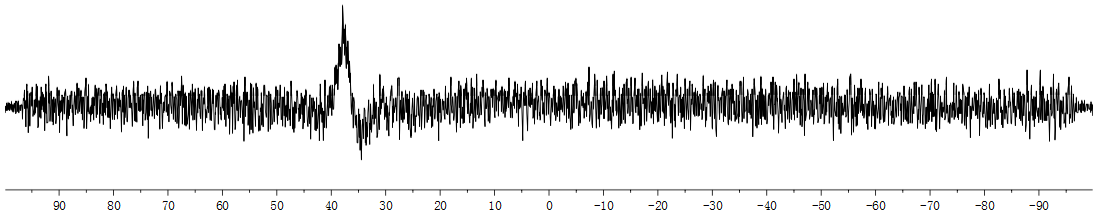


Figure S32. ^{11}B NMR spectra of **8** in $CDCl_3$**.**

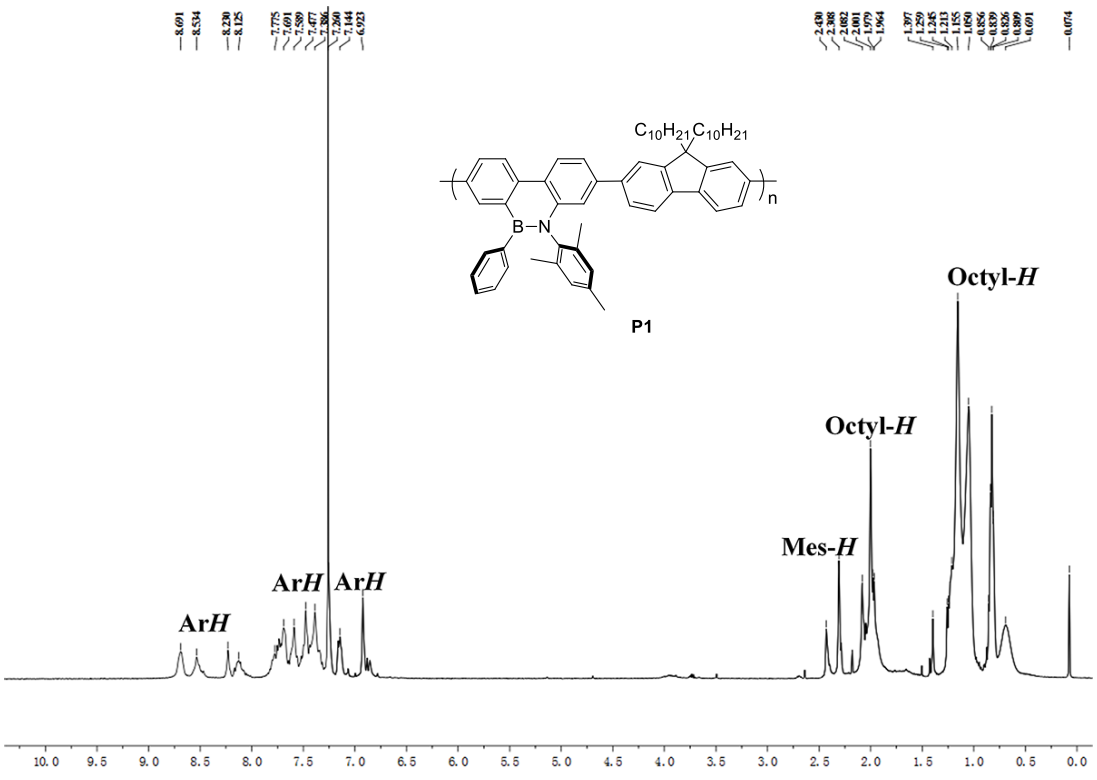


Figure S33. ^{1}H NMR spectra of **P1**in $CDCl_3$**.**

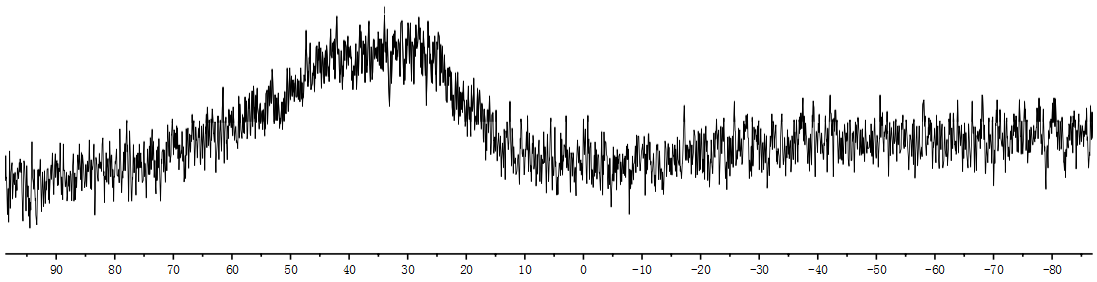


Figure S34. ^{11}B NMR spectra of **P1**in $CDCl_3$**.**

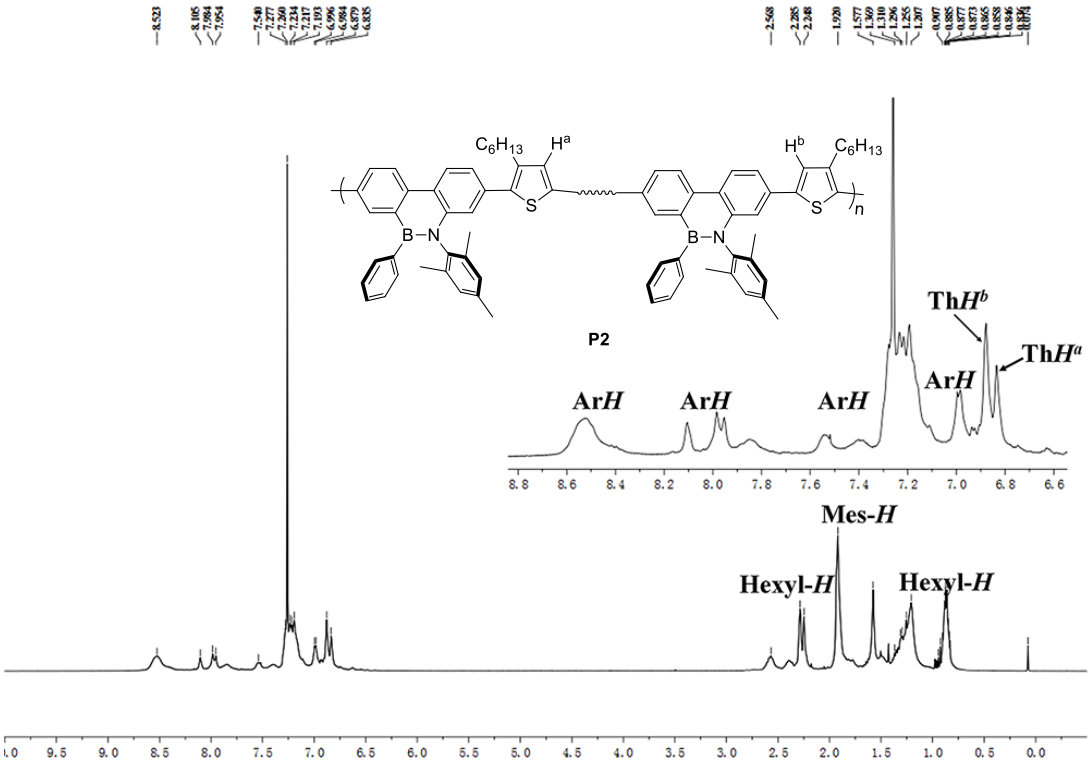


Figure S35. ^{1}H NMR spectra of **P2** in $CDCl_3$**.**

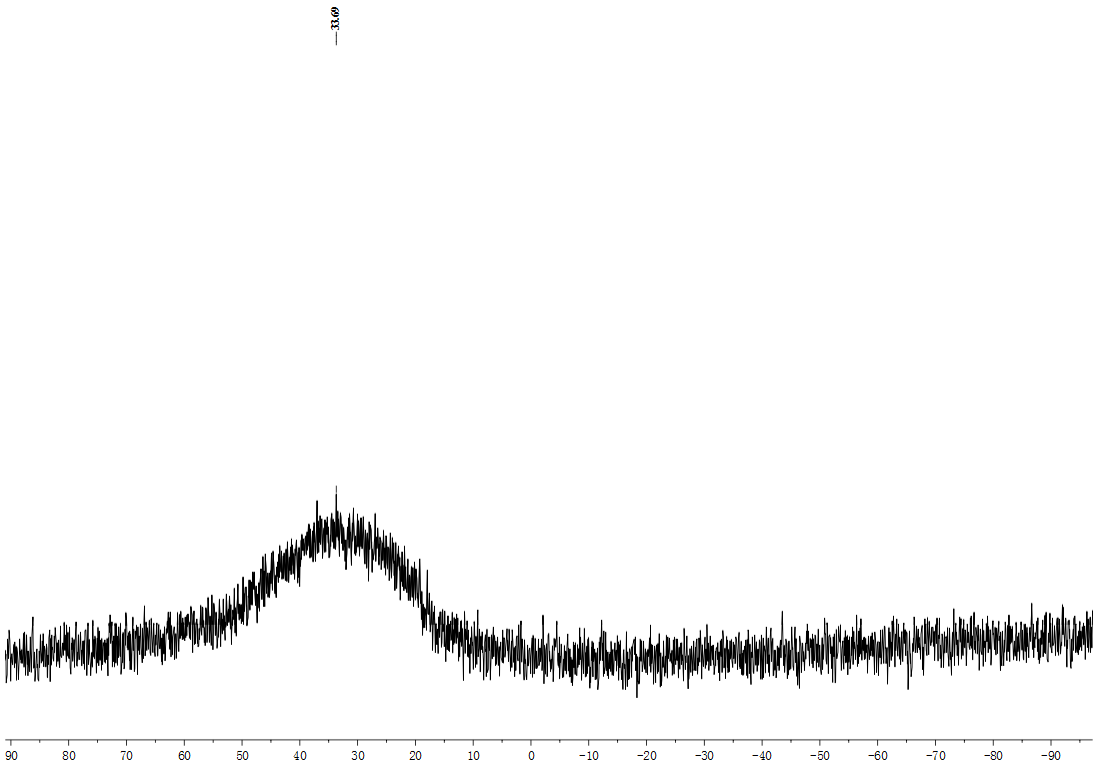


Figure S36. ^{11}B NMR spectra of **P2**in $CDCl_3$**.**

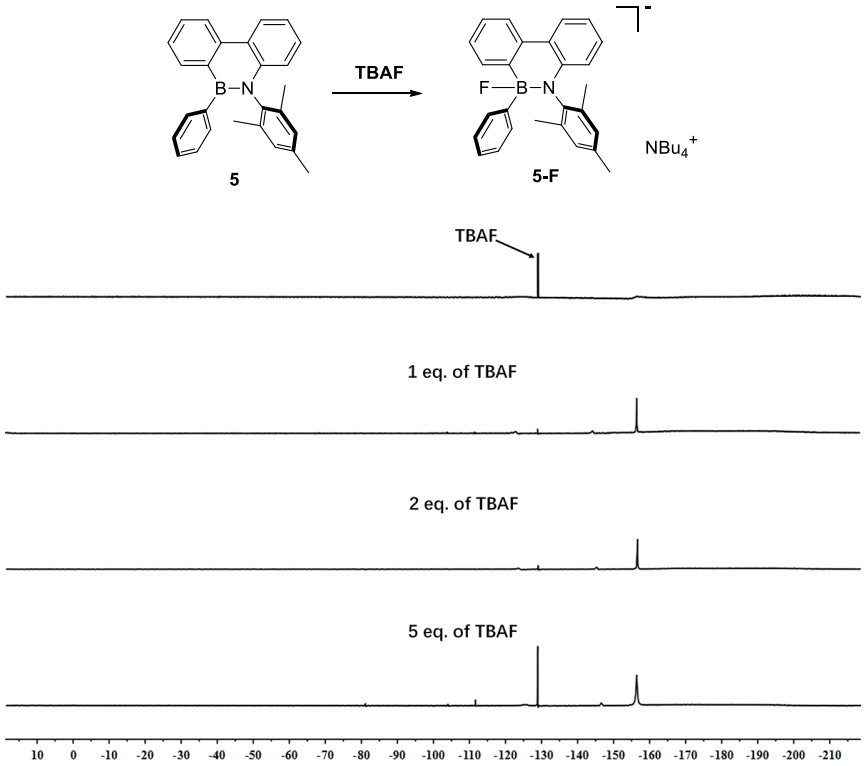


Figure S37. (top) Fluoride anion binding to model compound **5**. (bottom) ^{19}F NMR spectra of a mixture of **5** after addition of 1, 2 and 5 equivs. of TBAF.

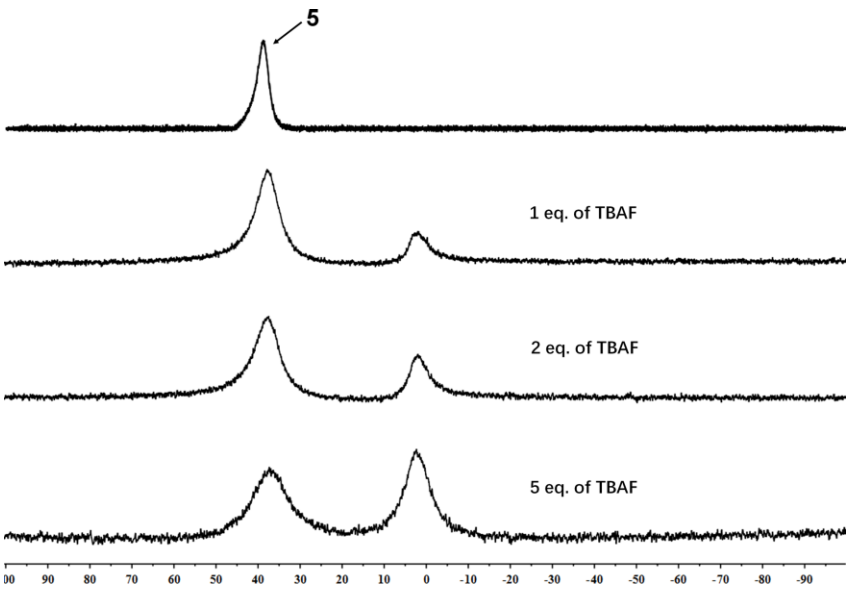


Figure S38. ^{11}B NMR spectra of a mixture of **5** after addition of 1, 2 and 5 equivs. of TBAF.

12. Coordinates of molecular structures

Table S17 Cartesian coordinates of optimized geometry of **5** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.731201	2.304305	0.288386
2	6	0	-2.160123	1.023901	0.119097
3	6	0	-3.020631	-0.105185	0.067557
4	6	0	-4.413698	0.095982	0.183375
5	6	0	-4.944051	1.367664	0.339832
6	6	0	-4.101754	2.485903	0.394272
7	6	0	-1.026830	-1.628372	-0.121629
8	6	0	-0.502967	-2.927885	-0.280011
9	6	0	-1.334185	-4.030055	-0.410465
10	6	0	-2.721741	-3.863714	-0.390834
11	6	0	-3.248163	-2.591215	-0.238463
12	6	0	-2.438167	-1.444610	-0.096787
13	5	0	-0.626649	0.828100	0.049598
14	7	0	-0.151721	-0.521877	-0.011402
15	6	0	0.365284	2.060188	0.021809
16	6	0	1.270671	-0.804236	0.011191
17	6	0	0.253322	3.005728	-1.018401
18	6	0	1.091297	4.120083	-1.093746
19	6	0	2.057286	4.333558	-0.109816
20	6	0	2.178839	3.422582	0.940894
21	6	0	1.349171	2.302201	0.998267
22	6	0	1.882956	-1.147584	1.230609
23	6	0	3.259976	-1.391462	1.238003
24	6	0	4.032208	-1.314657	0.075248
25	6	0	3.388260	-0.986574	-1.120532
26	6	0	2.013732	-0.732662	-1.179367
27	6	0	1.360898	-0.387276	-2.496188
28	6	0	1.083280	-1.266079	2.507323
29	6	0	5.514223	-1.609200	0.104956
30	1	0	-2.072718	3.165662	0.343792
31	1	0	-5.097766	-0.744915	0.162289
32	1	0	-6.020692	1.491223	0.427974

33	1	0	-4.518514	3.480964	0.525542
34	1	0	0.570904	-3.064906	-0.306010
35	1	0	-0.897717	-5.017576	-0.533278
36	1	0	-3.384301	-4.717761	-0.497823
37	1	0	-4.326245	-2.480144	-0.238619
38	1	0	-0.506161	2.867140	-1.785372
39	1	0	0.984380	4.823327	-1.916148
40	1	0	2.707420	5.203446	-0.159275
41	1	0	2.924335	3.582140	1.716139
42	1	0	1.473403	1.605889	1.822524
43	1	0	3.740421	-1.647237	2.180381
44	1	0	3.969490	-0.925219	-2.038525
45	1	0	0.448040	-0.969764	-2.660541
46	1	0	1.082563	0.672605	-2.535219
47	1	0	2.044449	-0.583286	-3.327939
48	1	0	0.514284	-0.354417	2.722537
49	1	0	0.354135	-2.083084	2.448430
50	1	0	1.741474	-1.463387	3.358715
51	1	0	5.714940	-2.668757	-0.103590
52	1	0	6.054187	-1.023554	-0.646746
53	1	0	5.947624	-1.383716	1.085093

Zero-point correction=	0.438133
Thermal correction to Energy=	0.462754
Thermal correction to Enthalpy=	0.463698
Thermal correction to Gibbs Free Energy=	0.382933
Sum of electronic and zero-point Energies=	-1122.596548
Sum of electronic and thermal Energies=	-1122.571927
Sum of electronic and thermal Enthalpies=	-1122.570983
Sum of electronic and thermal Free Energies=	-1122.651747

Table S18 Cartesian coordinates of optimized geometry of **5-F** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.964108	0.984002	-1.768501
2	6	0	2.140908	0.243531	-0.904056
3	6	0	2.697128	-0.872608	-0.240565
4	6	0	4.049071	-1.208615	-0.480232
5	6	0	4.845166	-0.448003	-1.328873
6	6	0	4.302239	0.663509	-1.981475
7	6	0	0.411449	-1.539665	0.623339
8	6	0	-0.357778	-2.490335	1.348651
9	6	0	0.228967	-3.480374	2.125530
10	6	0	1.618781	-3.577217	2.215698
11	6	0	2.390210	-2.690680	1.468290
12	6	0	1.840839	-1.698560	0.640931
13	5	0	0.596494	0.686264	-0.733894
14	7	0	-0.191307	-0.511744	-0.069198
15	6	0	0.459744	2.081540	0.123657
16	6	0	-1.618484	-0.531236	-0.215945
17	6	0	1.166090	2.305529	1.320623
18	6	0	1.041286	3.490689	2.048671
19	6	0	0.198239	4.507959	1.591617
20	6	0	-0.505096	4.321861	0.399432
21	6	0	-0.367556	3.129424	-0.317947
22	6	0	-2.177876	-1.131307	-1.367246
23	6	0	-3.564550	-1.120725	-1.541351
24	6	0	-4.423875	-0.540045	-0.604131
25	6	0	-3.855450	0.016184	0.541864
26	6	0	-2.470306	0.031850	0.757612
27	6	0	-1.933627	0.624881	2.039694
28	6	0	-1.292618	-1.792403	-2.395979
29	6	0	-5.918517	-0.507276	-0.832018
30	1	0	2.528440	1.836271	-2.286727
31	1	0	4.483046	-2.093851	-0.024000
32	1	0	5.883892	-0.731432	-1.492828
33	1	0	4.916220	1.262019	-2.653028
34	1	0	-1.439015	-2.424452	1.304850
35	1	0	-0.409644	-4.170491	2.675156

36	1	0	2.092839	-4.327374	2.844237
37	1	0	3.471548	-2.771344	1.532570
38	1	0	1.833778	1.528912	1.691303
39	1	0	1.603410	3.624811	2.972349
40	1	0	0.096369	5.434742	2.154361
41	1	0	-1.159968	5.109500	0.027074
42	1	0	-0.911856	2.996675	-1.249743
43	1	0	-3.983749	-1.583131	-2.434776
44	1	0	-4.505436	0.450565	1.301170
45	1	0	-1.102599	0.034997	2.435796
46	1	0	-1.558364	1.640616	1.883921
47	1	0	-2.723306	0.665394	2.799742
48	1	0	-0.616160	-1.054252	-2.833616
49	1	0	-0.670877	-2.572996	-1.942089
50	1	0	-1.894460	-2.250702	-3.189763
51	1	0	-6.466958	-0.430099	0.114184
52	1	0	-6.216769	0.352324	-1.449384
53	1	0	-6.267421	-1.409046	-1.350118
54	9	0	0.018087	0.933532	-2.031169

Zero-point correction=	0.437846
Thermal correction to Energy=	0.463663
Thermal correction to Enthalpy=	0.464607
Thermal correction to Gibbs Free Energy=	0.381416
Sum of electronic and zero-point Energies=	-1222.522263
Sum of electronic and thermal Energies=	-1222.496446
Sum of electronic and thermal Enthalpies=	-1222.495502
Sum of electronic and thermal Free Energies=	-1222.578693

Table S19 Cartesian coordinates of optimized geometry of **5-F'** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.964058	0.983819	-1.768685
2	6	0	-2.140871	0.243450	-0.904141
3	6	0	-2.697082	-0.872656	-0.240586
4	6	0	-4.049001	-1.208725	-0.480282
5	6	0	-4.845089	-0.448206	-1.329018
6	6	0	-4.302171	0.663269	-1.981688
7	6	0	-0.411406	-1.539614	0.623396
8	6	0	0.357823	-2.490232	1.348784
9	6	0	-0.228924	-3.480212	2.125735
10	6	0	-1.618739	-3.577047	2.215913
11	6	0	-2.390169	-2.690573	1.468434
12	6	0	-1.840796	-1.698519	0.640995
13	5	0	-0.596489	0.686261	-0.733931
14	7	0	0.191335	-0.511736	-0.069215
15	6	0	-0.459827	2.081518	0.123647
16	6	0	1.618512	-0.531195	-0.215966
17	6	0	0.367379	3.129472	-0.317954
18	6	0	0.504854	4.321904	0.399455
19	6	0	-0.198463	4.507920	1.591659
20	6	0	-1.041431	3.490574	2.048708
21	6	0	-1.166170	2.305430	1.320633
22	6	0	2.470335	0.031938	0.757568
23	6	0	3.855477	0.016261	0.541821
24	6	0	4.423904	-0.540012	-0.604154
25	6	0	3.564580	-1.120730	-1.541353
26	6	0	2.177907	-1.131304	-1.367246
27	6	0	1.292644	-1.792452	-2.395944
28	6	0	1.933656	0.625016	2.039631
29	6	0	5.918542	-0.507236	-0.832043
30	1	0	-2.528394	1.836057	-2.286968
31	1	0	-4.482961	-2.093944	-0.024005
32	1	0	-5.883799	-0.731686	-1.492986
33	1	0	-4.916137	1.261705	-2.653318
34	1	0	1.439059	-2.424349	1.304989
35	1	0	0.409685	-4.170286	2.675415

36	1	0	-2.092792	-4.327158	2.844509
37	1	0	-3.471508	-2.771220	1.532725
38	1	0	0.911665	2.996800	-1.249770
39	1	0	1.159661	5.109592	0.027090
40	1	0	-0.096655	5.434693	2.154428
41	1	0	-1.603541	3.624636	2.972401
42	1	0	-1.833800	1.528756	1.691301
43	1	0	4.505465	0.450671	1.301110
44	1	0	3.983781	-1.583170	-2.434760
45	1	0	0.670922	-2.573037	-1.942014
46	1	0	0.616176	-1.054326	-2.833608
47	1	0	1.894484	-2.250774	-3.189717
48	1	0	1.558530	1.640800	1.883843
49	1	0	1.102537	0.035227	2.435681
50	1	0	2.723302	0.665427	2.799718
51	1	0	6.466985	-0.430063	0.114158
52	1	0	6.267449	-1.408999	-1.350153
53	1	0	6.216790	0.352372	-1.449402
54	9	0	-0.018034	0.933552	-2.031159

Zero-point correction = 0.437848
Thermal correction to Energy= 0.463664
Thermal correction to Enthalpy= 0.464608
Thermal correction to Gibbs Free Energy= 0.381423
Sum of electronic and zero-point Energies= -1222.522262
Sum of electronic and thermal Energies= -1222.496446
Sum of electronic and thermal Enthalpies= -1222.495502
Sum of electronic and thermal Free Energies= -1222.578687

Table S20 Cartesian coordinates of optimized geometry of **8** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.154920	-0.566644	0.020526
2	6	0	-1.749390	-0.653179	-0.025162
3	6	0	-1.141076	-1.936105	-0.018166
4	6	0	-1.976532	-3.073559	0.028440
5	6	0	-3.354603	-2.953197	0.065224
6	6	0	-3.982077	-1.690187	0.063817
7	6	0	1.137966	-0.875236	-0.011860
8	6	0	2.538239	-1.012124	-0.030798
9	6	0	3.167400	-2.256621	-0.089810
10	6	0	2.355591	-3.404761	-0.135351
11	6	0	0.978377	-3.284971	-0.116406
12	6	0	0.320308	-2.039180	-0.048707
13	5	0	-0.863118	0.616682	-0.034652
14	7	0	0.553988	0.413567	0.030645
15	6	0	-1.489917	2.065164	-0.140114
16	6	0	1.456694	1.546458	0.104399
17	6	0	-2.291454	2.385087	-1.255409
18	6	0	-2.881922	3.641962	-1.401410
19	6	0	-2.704985	4.613868	-0.416091
20	6	0	-1.930323	4.318696	0.707011
21	6	0	-1.328529	3.066364	0.835474
22	6	0	1.944969	1.955514	1.359132
23	6	0	2.803873	3.057606	1.411285
24	6	0	3.190382	3.750962	0.260317
25	6	0	2.704885	3.302809	-0.970668
26	6	0	1.841507	2.206722	-1.074798
27	6	0	1.346084	1.755326	-2.427808
28	6	0	1.577914	1.217864	2.625932
29	6	0	4.092028	4.960341	0.347503
30	1	0	-3.610630	0.418196	0.003929
31	1	0	-1.552376	-4.071166	0.057963
32	1	0	-3.962377	-3.851780	0.130220
33	1	0	3.149339	-0.120601	0.025969
34	1	0	2.808675	-4.387901	-0.218432
35	1	0	0.388371	-4.192370	-0.174251

36	1	0	-2.458578	1.634191	-2.025029
37	1	0	-3.485543	3.857609	-2.279632
38	1	0	-3.168902	5.591456	-0.520578
39	1	0	-1.790075	5.066797	1.483505
40	1	0	-0.722948	2.869231	1.715185
41	1	0	3.182700	3.379452	2.379355
42	1	0	3.005524	3.818142	-1.880767
43	1	0	1.460516	0.674225	-2.562202
44	1	0	0.282592	1.988286	-2.558387
45	1	0	1.897874	2.258441	-3.227742
46	1	0	0.492552	1.146377	2.760781
47	1	0	1.960912	0.190462	2.615849
48	1	0	1.994949	1.723388	3.501978
49	1	0	4.783749	4.885885	1.193540
50	1	0	4.684701	5.085316	-0.564978
51	1	0	3.509129	5.881023	0.484613
52	6	0	4.648091	-2.361430	-0.107811
53	6	0	5.436667	-1.415764	-0.785663
54	6	0	5.301913	-3.414407	0.555366
55	6	0	6.826749	-1.518335	-0.798233
56	1	0	4.953465	-0.607736	-1.327539
57	6	0	6.691907	-3.517875	0.542357
58	1	0	4.715045	-4.142867	1.107864
59	6	0	7.461445	-2.570010	-0.134579
60	1	0	7.414927	-0.779100	-1.335838
61	1	0	7.174910	-4.336533	1.069619
62	1	0	8.545093	-2.650308	-0.145259
63	6	0	-5.460222	-1.566282	0.113188
64	6	0	-6.286617	-2.484628	-0.557402
65	6	0	-6.075208	-0.526278	0.831862
66	6	0	-7.675048	-2.367905	-0.511848
67	1	0	-5.835341	-3.282069	-1.141554
68	6	0	-7.463269	-0.408003	0.876239
69	1	0	-5.458481	0.180867	1.379283
70	6	0	-8.270487	-1.328592	0.205241
71	1	0	-8.292583	-3.085953	-1.045378
72	1	0	-7.915257	0.400914	1.444437
73	1	0	-9.352724	-1.237066	0.240907

Zero-point correction=	0.599927
Thermal correction to Energy=	0.634159
Thermal correction to Enthalpy=	0.635103
Thermal correction to Gibbs Free Energy=	0.531339
Sum of electronic and zero-point Energies=	-1584.550323
Sum of electronic and thermal Energies=	-1584.516091
Sum of electronic and thermal Enthalpies=	-1584.515147
Sum of electronic and thermal Free Energies=	-1584.618911

Table S21 Cartesian coordinates of optimized geometry of **8-F** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.212784	-0.313262	-0.283718
2	6	0	1.830172	-0.420778	-0.084794
3	6	0	1.273828	-1.706534	0.095567
4	6	0	2.132868	-2.828682	0.055975
5	6	0	3.499870	-2.689940	-0.127665
6	6	0	4.076555	-1.417332	-0.302440
7	6	0	-1.065150	-0.747731	-0.009364
8	6	0	-2.460012	-1.013840	-0.017352
9	6	0	-3.003812	-2.257796	0.311143
10	6	0	-2.131213	-3.302910	0.660292
11	6	0	-0.760790	-3.080843	0.622514
12	6	0	-0.184724	-1.853514	0.258865
13	5	0	0.938716	0.927802	-0.097248
14	7	0	-0.579584	0.513534	-0.261948
15	6	0	1.196028	1.837784	1.243579
16	6	0	-1.496147	1.523733	-0.711230
17	6	0	1.250700	1.280641	2.534927
18	6	0	1.459210	2.060874	3.674194
19	6	0	1.629318	3.443012	3.554121
20	6	0	1.595389	4.023924	2.284394
21	6	0	1.386956	3.228026	1.153901
22	6	0	-1.661332	1.724034	-2.100886
23	6	0	-2.519431	2.731522	-2.549808
24	6	0	-3.231078	3.546774	-1.664909
25	6	0	-3.080822	3.309810	-0.298704
26	6	0	-2.228599	2.313886	0.198769
27	6	0	-2.144345	2.104012	1.693241
28	6	0	-0.934578	0.852074	-3.096346
29	6	0	-4.126223	4.654395	-2.173326
30	1	0	3.629513	0.684370	-0.402882
31	1	0	1.727153	-3.833619	0.128177
32	1	0	4.122859	-3.579913	-0.185712
33	1	0	-3.128512	-0.212839	-0.309088
34	1	0	-2.519780	-4.262559	0.989186
35	1	0	-0.104773	-3.900371	0.900648

36	1	0	1.127813	0.204624	2.650923
37	1	0	1.492937	1.592489	4.657160
38	1	0	1.793259	4.057265	4.438106
39	1	0	1.735539	5.099057	2.175532
40	1	0	1.370819	3.687551	0.168678
41	1	0	-2.637323	2.879090	-3.622932
42	1	0	-3.645966	3.913224	0.411226
43	1	0	-2.034299	1.046465	1.946538
44	1	0	-1.282999	2.625732	2.121670
45	1	0	-3.049206	2.485532	2.181779
46	1	0	0.145039	0.972854	-2.979073
47	1	0	-1.161969	-0.208536	-2.936508
48	1	0	-1.220572	1.112463	-4.122097
49	1	0	-4.614275	4.377500	-3.115673
50	1	0	-4.910508	4.900648	-1.448071
51	1	0	-3.560438	5.577578	-2.363983
52	6	0	-4.473775	-2.464296	0.304311
53	6	0	-5.362622	-1.434240	0.663975
54	6	0	-5.030237	-3.703933	-0.062485
55	6	0	-6.742345	-1.633004	0.653229
56	1	0	-4.959975	-0.474292	0.973055
57	6	0	-6.409577	-3.906122	-0.068496
58	1	0	-4.367258	-4.507833	-0.369710
59	6	0	-7.276118	-2.870926	0.288540
60	1	0	-7.403245	-0.817967	0.940053
61	1	0	-6.809414	-4.873878	-0.364252
62	1	0	-8.352442	-3.026405	0.281636
63	6	0	5.535784	-1.260475	-0.509699
64	6	0	6.460429	-2.120390	0.112839
65	6	0	6.050724	-0.246187	-1.339401
66	6	0	7.832799	-1.977501	-0.086595
67	1	0	6.094057	-2.894205	0.781855
68	6	0	7.422751	-0.098230	-1.534837
69	1	0	5.360028	0.418997	-1.849200
70	6	0	8.324517	-0.964135	-0.911853
71	1	0	8.521677	-2.654201	0.414934
72	1	0	7.788750	0.693349	-2.185186
73	1	0	9.394943	-0.849334	-1.065718
74	9	0	1.303951	1.733556	-1.233778

Zero-point correction= 0.599872

Thermal correction to Energy=	0.635222
Thermal correction to Enthalpy=	0.636166
Thermal correction to Gibbs Free Energy=	0.530519
Sum of electronic and zero-point Energies=	-1684.481502
Sum of electronic and thermal Energies=	-1684.446152
Sum of electronic and thermal Enthalpies=	-1684.445208
Sum of electronic and thermal Free Energies=	-1684.550855

Table S22 Cartesian coordinates of optimized geometry of **8-F'** (DFT, B3LYP/6-31g*) Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.062461	-0.689977	-0.282703
2	6	0	-1.667987	-0.731338	-0.403423
3	6	0	-1.012719	-1.949292	-0.101087
4	6	0	-1.776137	-3.053322	0.334880
5	6	0	-3.157655	-2.980266	0.438041
6	6	0	-3.836349	-1.788220	0.124212
7	6	0	1.234874	-0.818828	-0.205928
8	6	0	2.643230	-0.946148	-0.148482
9	6	0	3.294993	-2.182856	-0.142479
10	6	0	2.516783	-3.352818	-0.200538
11	6	0	1.132249	-3.250523	-0.228447
12	6	0	0.454403	-2.021536	-0.197986
13	5	0	-0.801060	0.536618	-0.935401
14	7	0	0.620648	0.420748	-0.255527
15	6	0	-1.524653	1.968204	-0.620710
16	6	0	1.391122	1.559843	0.129764
17	6	0	-1.956481	2.785290	-1.680734
18	6	0	-2.631089	3.991325	-1.467635
19	6	0	-2.904376	4.420193	-0.168097
20	6	0	-2.499163	3.625454	0.907597
21	6	0	-1.826296	2.423957	0.676392
22	6	0	1.646026	1.783013	1.505500
23	6	0	2.370081	2.910629	1.898259
24	6	0	2.864156	3.833160	0.971105
25	6	0	2.627335	3.582706	-0.380138
26	6	0	1.905146	2.466112	-0.822773
27	6	0	1.716819	2.258645	-2.306537
28	6	0	1.160240	0.808053	2.551406
29	6	0	3.611518	5.067908	1.421423
30	1	0	-3.568093	0.236201	-0.544125
31	1	0	-1.282273	-3.972583	0.638743
32	1	0	-3.712072	-3.837611	0.813748
33	1	0	3.234363	-0.038542	-0.100760
34	1	0	2.992358	-4.327562	-0.265059

35	1	0	0.548153	-4.164428	-0.293433
36	1	0	-1.758887	2.450428	-2.695863
37	1	0	-2.947604	4.595269	-2.317410
38	1	0	-3.429965	5.357719	0.005985
39	1	0	-2.708657	3.943703	1.928076
40	1	0	-1.533374	1.818844	1.532186
41	1	0	2.549118	3.073893	2.960793
42	1	0	3.022036	4.273422	-1.124994
43	1	0	1.663458	1.199680	-2.564624
44	1	0	0.774332	2.699957	-2.648886
45	1	0	2.534573	2.732571	-2.863462
46	1	0	0.137818	0.477939	2.345258
47	1	0	1.779787	-0.098023	2.570385
48	1	0	1.193349	1.258933	3.549660
49	1	0	4.258240	4.857734	2.282230
50	1	0	4.241066	5.469318	0.618789
51	1	0	2.923634	5.869940	1.725092
52	6	0	4.776803	-2.257926	-0.099831
53	6	0	5.581333	-1.297141	-0.739978
54	6	0	5.429704	-3.299887	0.584954
55	6	0	6.972606	-1.372562	-0.694029
56	1	0	5.104646	-0.495409	-1.296010
57	6	0	6.820844	-3.379702	0.627634
58	1	0	4.832171	-4.040506	1.109125
59	6	0	7.602770	-2.415151	-0.011169
60	1	0	7.567057	-0.616838	-1.202782
61	1	0	7.295826	-4.193586	1.171544
62	1	0	8.688092	-2.474642	0.023144
63	6	0	-5.311425	-1.693903	0.239662
64	6	0	-6.140056	-2.799365	-0.030691
65	6	0	-5.936699	-0.493509	0.628304
66	6	0	-7.526650	-2.712648	0.086169
67	1	0	-5.687054	-3.730335	-0.360615
68	6	0	-7.323135	-0.403918	0.739471
69	1	0	-5.321469	0.370420	0.861847
70	6	0	-8.128742	-1.513207	0.471731
71	1	0	-8.140042	-3.583471	-0.136354
72	1	0	-7.775707	0.536761	1.045574
73	1	0	-9.210409	-1.443201	0.560394
74	9	0	-0.643275	0.409220	-2.364571

Zero-point correction=	0.599696
Thermal correction to Energy=	0.635185
Thermal correction to Enthalpy=	0.636129
Thermal correction to Gibbs Free Energy=	0.530053
Sum of electronic and zero-point Energies=	-1684.481092
Sum of electronic and thermal Energies=	-1684.445603
Sum of electronic and thermal Enthalpies=	-1684.444659
Sum of electronic and thermal Free Energies=	-1684.550735

Table S23. Cartesian coordinates of optimized geometry of P1 (DFT, B3LYP/6-31g*) Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.624544	1.671702	3.651334
2	6	0	5.717938	0.954925	2.840026
3	6	0	4.337422	0.988737	3.164979
4	6	0	3.931017	1.736394	4.292703
5	6	0	4.851105	2.419457	5.069308
6	6	0	6.225062	2.403157	4.763849
7	6	0	3.382388	0.258636	2.325640
8	6	0	3.808231	-0.418050	1.148837
9	6	0	2.864808	-1.109427	0.366470
10	6	0	1.510130	-1.163278	0.700528
11	6	0	1.093592	-0.494178	1.866502
12	6	0	2.010324	0.188338	2.644491
13	5	0	6.190424	0.187577	1.581813
14	7	0	5.172490	-0.411889	0.770514
15	6	0	7.725377	0.044524	1.225572
16	6	0	5.517570	-1.073929	-0.472679
17	6	0	8.309532	0.523587	0.038510
18	6	0	9.676383	0.392872	-0.210096
19	6	0	10.502691	-0.238220	0.721421
20	6	0	9.952074	-0.724506	1.907662
21	6	0	8.586608	-0.572340	2.156336
22	6	0	5.389485	-0.368614	-1.683770
23	6	0	5.741303	-1.016895	-2.871457
24	6	0	6.205995	-2.335593	-2.885784
25	6	0	6.298690	-3.012988	-1.667585
26	6	0	5.959704	-2.407292	-0.452479
27	6	0	4.865124	1.048202	-1.717256
28	6	0	6.067851	-3.181769	0.839196
29	6	0	6.612897	-3.001174	-4.179923
30	6	0	0.544531	-1.910292	-0.142668
31	6	0	0.912384	-3.115870	-0.768614
32	6	0	0.004590	-3.837561	-1.540595
33	6	0	-1.292139	-3.347436	-1.705733
34	6	0	-1.674439	-2.127527	-1.111888

35	6	0	-0.768509	-1.428860	-0.322763
36	6	0	-2.442009	-3.901725	-2.421325
37	6	0	-2.570376	-5.068380	-3.175689
38	6	0	-3.792883	-5.349914	-3.786222
39	6	0	-4.886481	-4.480489	-3.664965
40	6	0	-4.738686	-3.305875	-2.906812
41	6	0	-3.534485	-3.023240	-2.269851
42	6	0	-3.141961	-1.801369	-1.426387
43	6	0	7.214689	3.160832	5.616461
44	6	0	-6.208959	-4.805578	-4.320782
45	6	0	-13.865097	0.024352	5.545753
46	6	0	-12.358054	-0.251638	5.535532
47	6	0	-11.764277	-0.324967	4.123040
48	6	0	-10.255054	-0.599680	4.105607
49	6	0	-9.658657	-0.676134	2.694319
50	6	0	-8.149051	-0.950194	2.683499
51	6	0	-7.546687	-1.036187	1.275265
52	6	0	-6.037483	-1.312852	1.276120
53	6	0	-5.426937	-1.416274	-0.129299
54	6	0	-3.921779	-1.713591	-0.077938
55	6	0	-2.345259	10.944533	-3.346370
56	6	0	-2.787370	9.583185	-3.892858
57	6	0	-2.507291	8.423035	-2.928885
58	6	0	-2.942101	7.055483	-3.470938
59	6	0	-2.658869	5.894186	-2.509165
60	6	0	-3.084335	4.526297	-3.058253
61	6	0	-2.798807	3.362943	-2.099589
62	6	0	-3.208269	1.994748	-2.659947
63	6	0	-2.923284	0.829046	-1.701029
64	6	0	-3.304059	-0.526587	-2.312138
65	1	0	7.678637	1.654622	3.388145
66	1	0	2.883847	1.798308	4.568007
67	1	0	4.501525	2.987097	5.929862
68	1	0	3.198151	-1.600513	-0.538786
69	1	0	0.054949	-0.542356	2.178985
70	1	0	1.651715	0.669677	3.547089
71	1	0	7.689388	1.009569	-0.709176
72	1	0	10.096072	0.780599	-1.135209
73	1	0	11.566522	-0.346845	0.525608
74	1	0	10.585096	-1.215718	2.642754
75	1	0	8.179085	-0.940695	3.095661

76	1	0	5.646346	-0.475496	-3.810697
77	1	0	6.642501	-4.045437	-1.657922
78	1	0	3.824748	1.097302	-1.374498
79	1	0	5.441138	1.715294	-1.065665
80	1	0	4.903724	1.450965	-2.733803
81	1	0	6.232939	-4.244799	0.638437
82	1	0	6.906296	-2.822785	1.447889
83	1	0	5.161062	-3.085507	1.445996
84	1	0	6.010957	-2.643465	-5.022354
85	1	0	7.664017	-2.792448	-4.420513
86	1	0	6.503276	-4.089329	-4.122865
87	1	0	1.913336	-3.508842	-0.615749
88	1	0	0.304789	-4.780369	-1.991048
89	1	0	-1.053893	-0.495502	0.152074
90	1	0	-1.729891	-5.746916	-3.299219
91	1	0	-3.899547	-6.256176	-4.378257
92	1	0	-5.577891	-2.618453	-2.837666
93	1	0	8.232387	3.063920	5.225721
94	1	0	6.972729	4.230502	5.658568
95	1	0	7.217431	2.793476	6.650897
96	1	0	-6.706232	-3.902172	-4.691624
97	1	0	-6.080276	-5.490606	-5.165389
98	1	0	-6.899320	-5.286064	-3.614022
99	1	0	-14.257700	0.068043	6.568172
100	1	0	-14.096770	0.979988	5.059207
101	1	0	-14.415464	-0.759688	5.011025
102	1	0	-12.155414	-1.195021	6.062505
103	1	0	-11.838828	0.531670	6.106086
104	1	0	-11.968784	0.618672	3.595107
105	1	0	-12.283565	-1.109421	3.552249
106	1	0	-10.052016	-1.542155	4.635881
107	1	0	-9.737228	0.185739	4.676205
108	1	0	-9.861288	0.265615	2.162643
109	1	0	-10.174681	-1.462887	2.124015
110	1	0	-7.947562	-1.889180	3.220354
111	1	0	-7.633535	-0.161092	3.251031
112	1	0	-7.745489	-0.097760	0.736281
113	1	0	-8.060571	-1.826482	0.708040
114	1	0	-5.841342	-2.246598	1.823607
115	1	0	-5.523985	-0.518979	1.838806
116	1	0	-5.614628	-0.478963	-0.671052

117	1	0	-5.946659	-2.207322	-0.683633
118	1	0	-3.767060	-2.661222	0.454595
119	1	0	-3.437762	-0.944346	0.538418
120	1	0	-2.557599	11.750713	-4.057984
121	1	0	-2.863221	11.182923	-2.409080
122	1	0	-1.267875	10.957721	-3.139902
123	1	0	-2.279062	9.389894	-4.848341
124	1	0	-3.862261	9.612031	-4.121877
125	1	0	-3.017824	8.615377	-1.973229
126	1	0	-1.431933	8.397096	-2.697090
127	1	0	-2.432146	6.866036	-4.427352
128	1	0	-4.017587	7.081595	-3.701820
129	1	0	-3.173771	6.079397	-1.554601
130	1	0	-1.584385	5.871972	-2.273828
131	1	0	-2.569037	4.343081	-4.012948
132	1	0	-4.158869	4.547423	-3.293921
133	1	0	-3.322863	3.539257	-1.148255
134	1	0	-1.726136	3.348295	-1.856123
135	1	0	-2.680253	1.819472	-3.608957
136	1	0	-4.280082	2.009077	-2.908181
137	1	0	-3.471971	0.997363	-0.763877
138	1	0	-1.857098	0.835556	-1.443716
139	1	0	-2.712630	-0.680969	-3.224173
140	1	0	-4.350589	-0.479619	-2.641559

Zero-point correction=	1.232871
Thermal correction to Energy=	1.298682
Thermal correction to Enthalpy=	1.299626
Thermal correction to Gibbs Free Energy=	1.119448
Sum of electronic and zero-point Energies=	-2486.937755
Sum of electronic and thermal Energies=	-2486.871944
Sum of electronic and thermal Enthalpies=	-2486.871000
Sum of electronic and thermal Free Energies=	-2487.051178

Table S24 Cartesian coordinates of optimized geometry of **P1-F** (DFT, B3LYP/6-31g*) Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.480496	1.425235	3.660453
2	6	0	5.596591	0.625926	2.919495
3	6	0	4.210261	0.868731	3.063890
4	6	0	3.775225	1.913140	3.906623
5	6	0	4.680978	2.677883	4.630662
6	6	0	6.058979	2.437485	4.527385
7	6	0	3.251553	0.057805	2.292234
8	6	0	3.690666	-0.676097	1.141806
9	6	0	2.708992	-1.324340	0.356669
10	6	0	1.348113	-1.317393	0.681669
11	6	0	0.940680	-0.642993	1.846313
12	6	0	1.887402	0.017265	2.619503
13	5	0	6.102741	-0.591237	1.967827
14	7	0	5.035247	-0.732299	0.812403
15	6	0	7.613152	-0.355362	1.389485
16	6	0	5.373500	-1.099369	-0.524727
17	6	0	7.970484	0.717348	0.551563
18	6	0	9.282213	0.921920	0.119232
19	6	0	10.297374	0.050473	0.522601
20	6	0	9.978882	-1.017113	1.363256
21	6	0	8.659669	-1.207437	1.785963
22	6	0	5.171008	-0.158849	-1.565832
23	6	0	5.521438	-0.493095	-2.875344
24	6	0	6.066159	-1.739038	-3.200528
25	6	0	6.236061	-2.660556	-2.167813
26	6	0	5.900806	-2.371177	-0.837984
27	6	0	4.567400	1.195024	-1.277894
28	6	0	6.097574	-3.436893	0.213589
29	6	0	6.476042	-2.065366	-4.618862
30	6	0	0.362364	-2.025123	-0.169981
31	6	0	0.689549	-3.232247	-0.820954
32	6	0	-0.237460	-3.912419	-1.606650
33	6	0	-1.520468	-3.383675	-1.764570
34	6	0	-1.864702	-2.165139	-1.146684

35	6	0	-0.938957	-1.507011	-0.345439
36	6	0	-2.685080	-3.887640	-2.492239
37	6	0	-2.852992	-5.034023	-3.269526
38	6	0	-4.083612	-5.263678	-3.889000
39	6	0	-5.147590	-4.362476	-3.755580
40	6	0	-4.961993	-3.207983	-2.972973
41	6	0	-3.752300	-2.977727	-2.327591
42	6	0	-3.320580	-1.785318	-1.460412
43	6	0	7.050594	3.242929	5.336407
44	6	0	-6.477472	-4.624824	-4.425812
45	6	0	-14.027167	0.223809	5.489886
46	6	0	-12.525755	-0.081902	5.482368
47	6	0	-11.927177	-0.151879	4.071795
48	6	0	-10.423900	-0.457882	4.057314
49	6	0	-9.822538	-0.531741	2.648036
50	6	0	-8.319696	-0.841181	2.640224
51	6	0	-7.712557	-0.924977	1.233959
52	6	0	-6.211553	-1.243528	1.237128
53	6	0	-5.597512	-1.344973	-0.166731
54	6	0	-4.103169	-1.693798	-0.114828
55	6	0	-1.971458	10.945408	-3.139267
56	6	0	-2.454366	9.612988	-3.721594
57	6	0	-2.249467	8.425851	-2.771645
58	6	0	-2.726592	7.087176	-3.349063
59	6	0	-2.519984	5.899046	-2.400591
60	6	0	-2.987795	4.559738	-2.984643
61	6	0	-2.778075	3.370021	-2.038833
62	6	0	-3.229464	2.029233	-2.632360
63	6	0	-3.013519	0.838371	-1.686694
64	6	0	-3.437161	-0.491534	-2.325022
65	1	0	7.549351	1.246832	3.553124
66	1	0	2.717678	2.155785	3.974563
67	1	0	4.317296	3.482070	5.270320
68	1	0	3.033706	-1.837982	-0.541355
69	1	0	-0.097223	-0.674208	2.166611
70	1	0	1.556576	0.512828	3.528131
71	1	0	7.201660	1.418143	0.232260
72	1	0	9.514780	1.762645	-0.533254
73	1	0	11.322204	0.205091	0.188727
74	1	0	10.760013	-1.701745	1.692517
75	1	0	8.420592	-2.035056	2.449210

76	1	0	5.368573	0.244208	-3.663210
77	1	0	6.637225	-3.647348	-2.398602
78	1	0	3.484656	1.122238	-1.112373
79	1	0	4.988421	1.633246	-0.367956
80	1	0	4.735100	1.882656	-2.114613
81	1	0	6.012344	-4.434638	-0.234725
82	1	0	7.090378	-3.356933	0.671124
83	1	0	5.381365	-3.338347	1.030754
84	1	0	5.792296	-1.617584	-5.350508
85	1	0	7.482902	-1.687473	-4.847489
86	1	0	6.490976	-3.147765	-4.792206
87	1	0	1.679704	-3.653084	-0.676142
88	1	0	0.037567	-4.854583	-2.075751
89	1	0	-1.192900	-0.574374	0.148069
90	1	0	-2.034864	-5.737445	-3.404243
91	1	0	-4.217603	-6.155506	-4.498185
92	1	0	-5.777589	-2.493033	-2.892867
93	1	0	8.057724	3.176231	4.909988
94	1	0	6.772732	4.304259	5.380775
95	1	0	7.114312	2.887246	6.375461
96	1	0	-6.877766	-3.717996	-4.895535
97	1	0	-6.389728	-5.392615	-5.202129
98	1	0	-7.232684	-4.972068	-3.706909
99	1	0	-14.423788	0.263734	6.511142
100	1	0	-14.237794	1.189299	5.013108
101	1	0	-14.590542	-0.542990	4.943563
102	1	0	-12.344121	-1.034705	6.000007
103	1	0	-11.993625	0.684584	6.063692
104	1	0	-12.109941	0.801647	3.553569
105	1	0	-12.460349	-0.918964	3.490056
106	1	0	-10.243040	-1.410060	4.578229
107	1	0	-9.892247	0.310038	4.638789
108	1	0	-10.000933	0.420710	2.126615
109	1	0	-10.354436	-1.299460	2.066172
110	1	0	-8.143092	-1.790940	3.166816
111	1	0	-7.788223	-0.071681	3.219624
112	1	0	-7.883241	0.025795	0.706795
113	1	0	-8.245695	-1.693075	0.653715
114	1	0	-6.044285	-2.189856	1.772491
115	1	0	-5.678470	-0.472861	1.813325
116	1	0	-5.751454	-0.393180	-0.694166

117	1	0	-6.141221	-2.108958	-0.736346
118	1	0	-3.982773	-2.655082	0.401691
119	1	0	-3.594855	-0.953341	0.516584
120	1	0	-2.131525	11.772684	-3.840808
121	1	0	-2.503222	11.188236	-2.210757
122	1	0	-0.900388	10.909824	-2.904916
123	1	0	-1.927964	9.414858	-4.666269
124	1	0	-3.520571	9.690803	-3.979367
125	1	0	-2.776894	8.623856	-1.826309
126	1	0	-1.183066	8.350226	-2.512174
127	1	0	-2.198078	6.891851	-4.294197
128	1	0	-3.793314	7.163500	-3.609313
129	1	0	-3.052697	6.090781	-1.457090
130	1	0	-1.454789	5.826534	-2.136702
131	1	0	-2.453555	4.370283	-3.927685
132	1	0	-4.053764	4.630980	-3.249792
133	1	0	-3.319589	3.553689	-1.098657
134	1	0	-1.714570	3.305382	-1.767463
135	1	0	-2.684936	1.848108	-3.570939
136	1	0	-4.293854	2.091527	-2.906625
137	1	0	-3.574053	1.015987	-0.758102
138	1	0	-1.954473	0.795395	-1.407758
139	1	0	-2.842434	-0.650306	-3.234158
140	1	0	-4.479182	-0.402291	-2.662658
141	9	0	6.098250	-1.803809	2.752854

Zero-point correction= 1.232463
Thermal correction to Energy= 1.299535
Thermal correction to Enthalpy= 1.300479
Thermal correction to Gibbs Free Energy= 1.116536
Sum of electronic and zero-point Energies= -2586.865664
Sum of electronic and thermal Energies= -2586.798592
Sum of electronic and thermal Enthalpies= -2586.797648
Sum of electronic and thermal Free Energies= -2586.981592

Table S25 Cartesian coordinates of optimized geometry of **P1-F'** (DFT, B3LYP/6-31g*) Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.498676	2.557996	2.885106
2	6	0	5.700817	1.584339	2.271255
3	6	0	4.317803	1.565324	2.560843
4	6	0	3.796912	2.527905	3.449429
5	6	0	4.620104	3.470101	4.057736
6	6	0	5.994121	3.501859	3.785334
7	6	0	3.443934	0.591745	1.874115
8	6	0	3.917210	-0.121886	0.717139
9	6	0	2.963830	-0.866410	-0.025327
10	6	0	1.634075	-1.012656	0.378390
11	6	0	1.212855	-0.392819	1.566737
12	6	0	2.116150	0.390592	2.276558
13	5	0	6.383045	0.527201	1.258302
14	7	0	5.239259	-0.074650	0.340822
15	6	0	7.205308	-0.620404	2.093897
16	6	0	5.600323	-0.562067	-0.961483
17	6	0	8.558288	-0.886819	1.822087
18	6	0	9.284375	-1.846079	2.535439
19	6	0	8.671214	-2.569369	3.560371
20	6	0	7.329253	-2.316395	3.862585
21	6	0	6.618770	-1.356100	3.141096
22	6	0	5.578066	0.346860	-2.046968
23	6	0	5.956088	-0.090816	-3.316947
24	6	0	6.353309	-1.411319	-3.557184
25	6	0	6.343398	-2.298964	-2.483745
26	6	0	5.970439	-1.904115	-1.189449
27	6	0	5.141100	1.776498	-1.841156
28	6	0	5.963298	-2.943009	-0.093539
29	6	0	6.767301	-1.856052	-4.940604
30	6	0	0.687125	-1.819872	-0.429368
31	6	0	1.105565	-2.990781	-1.092199
32	6	0	0.214822	-3.763766	-1.833702
33	6	0	-1.119842	-3.364294	-1.930069
34	6	0	-1.556522	-2.180888	-1.300210

35	6	0	-0.664865	-1.432137	-0.540767
36	6	0	-2.261072	-3.988677	-2.599865
37	6	0	-2.347276	-5.151413	-3.364772
38	6	0	-3.575950	-5.508631	-3.926075
39	6	0	-4.716031	-4.715449	-3.748868
40	6	0	-4.614308	-3.543781	-2.974663
41	6	0	-3.408058	-3.191536	-2.381620
42	6	0	-3.059983	-1.958988	-1.531360
43	6	0	6.899134	4.521721	4.436610
44	6	0	-6.035366	-5.096924	-4.379145
45	6	0	-13.417147	-0.469030	6.018644
46	6	0	-11.916611	-0.765592	5.936866
47	6	0	-11.384530	-0.790193	4.498348
48	6	0	-9.881887	-1.083889	4.407955
49	6	0	-9.349969	-1.105204	2.969495
50	6	0	-7.846090	-1.393681	2.880046
51	6	0	-7.312747	-1.409043	1.441932
52	6	0	-5.806898	-1.687923	1.353397
53	6	0	-5.273573	-1.696626	-0.087010
54	6	0	-3.761433	-1.954405	-0.137926
55	6	0	-3.844299	10.845300	-2.815774
56	6	0	-4.108795	9.474716	-3.446701
57	6	0	-3.646693	8.306854	-2.566119
58	6	0	-3.909704	6.930121	-3.188915
59	6	0	-3.453076	5.764505	-2.302767
60	6	0	-3.718539	4.386406	-2.921822
61	6	0	-3.273594	3.223320	-2.026329
62	6	0	-3.538535	1.843384	-2.641784
63	6	0	-3.108080	0.683455	-1.732086
64	6	0	-3.375279	-0.684261	-2.374711
65	1	0	7.561475	2.573988	2.643785
66	1	0	2.729821	2.571872	3.649505
67	1	0	4.186878	4.200480	4.740485
68	1	0	3.283250	-1.334967	-0.949242
69	1	0	0.203506	-0.540840	1.939947
70	1	0	1.773598	0.865307	3.192154
71	1	0	9.044048	-0.325391	1.027628
72	1	0	10.330858	-2.027586	2.292949
73	1	0	9.230845	-3.316060	4.121037
74	1	0	6.839557	-2.868119	4.663861
75	1	0	5.576267	-1.170992	3.398692

76	1	0	5.936783	0.619700	-4.142974
77	1	0	6.626900	-3.338128	-2.649337
78	1	0	4.135754	1.829778	-1.406643
79	1	0	5.821110	2.276119	-1.145716
80	1	0	5.132820	2.322038	-2.792048
81	1	0	5.803595	-3.942915	-0.516033
82	1	0	6.914431	-2.955107	0.448932
83	1	0	5.181021	-2.746561	0.643009
84	1	0	5.990749	-1.637985	-5.685722
85	1	0	7.680820	-1.344311	-5.272791
86	1	0	6.963803	-2.933602	-4.970400
87	1	0	2.140352	-3.305675	-0.994279
88	1	0	0.557767	-4.678152	-2.312669
89	1	0	-0.985072	-0.534278	-0.021463
90	1	0	-1.470043	-5.770898	-3.534871
91	1	0	-3.646379	-6.414527	-4.525101
92	1	0	-5.492881	-2.912584	-2.863487
93	1	0	7.438626	5.118962	3.689399
94	1	0	6.332478	5.214543	5.070117
95	1	0	7.659743	4.042667	5.067973
96	1	0	-6.401999	-4.311868	-5.053486
97	1	0	-5.947233	-6.019872	-4.962280
98	1	0	-6.814097	-5.256485	-3.621706
99	1	0	-13.767220	-0.457421	7.057264
100	1	0	-13.653127	0.506917	5.576427
101	1	0	-14.000929	-1.224696	5.478409
102	1	0	-11.707263	-1.732196	6.418352
103	1	0	-11.362316	-0.012430	6.516019
104	1	0	-11.596672	0.176991	4.016802
105	1	0	-11.939548	-1.543996	3.918661
106	1	0	-9.670087	-2.051109	4.889148
107	1	0	-9.328688	-0.330193	4.989057
108	1	0	-9.563938	-0.138206	2.488627
109	1	0	-9.901540	-1.860115	2.388151
110	1	0	-7.631129	-2.361164	3.359064
111	1	0	-7.296237	-0.639396	3.463396
112	1	0	-7.532065	-0.442084	0.963256
113	1	0	-7.859444	-2.165946	0.858501
114	1	0	-5.585890	-2.655262	1.829322
115	1	0	-5.262851	-0.931799	1.939711
116	1	0	-5.513041	-0.732479	-0.559076

117	1	0	-5.808333	-2.465777	-0.658298
118	1	0	-3.544489	-2.915773	0.348271
119	1	0	-3.264037	-1.194139	0.479405
120	1	0	-4.183915	11.658842	-3.467348
121	1	0	-4.365384	10.947048	-1.855684
122	1	0	-2.774177	10.994399	-2.626281
123	1	0	-3.603074	9.416756	-4.421904
124	1	0	-5.183734	9.369009	-3.656144
125	1	0	-4.151207	8.367286	-1.589379
126	1	0	-2.571281	8.412983	-2.356940
127	1	0	-3.401452	6.868320	-4.163521
128	1	0	-4.985185	6.826695	-3.401830
129	1	0	-3.960685	5.828785	-1.327984
130	1	0	-2.378235	5.866926	-2.090402
131	1	0	-3.203423	4.317546	-3.892261
132	1	0	-4.793051	4.287161	-3.141899
133	1	0	-3.790046	3.294127	-1.056595
134	1	0	-2.200561	3.322608	-1.804846
135	1	0	-3.010310	1.766199	-3.604280
136	1	0	-4.610624	1.748464	-2.875822
137	1	0	-3.642092	0.766847	-0.774210
138	1	0	-2.040692	0.787352	-1.504304
139	1	0	-2.807567	-0.754667	-3.312918
140	1	0	-4.434865	-0.728341	-2.664436
141	9	0	7.323305	1.199944	0.408861

Zero-point correction=	1.232212
Thermal correction to Energy=	1.299424
Thermal correction to Enthalpy=	1.300368
Thermal correction to Gibbs Free Energy=	1.116239
Sum of electronic and zero-point Energies=	-2586.866641
Sum of electronic and thermal Energies=	-2586.799430
Sum of electronic and thermal Enthalpies=	-2586.798485
Sum of electronic and thermal Free Energies=	-2586.982615

Table S26 Cartesian coordinates of optimized geometry of **P2** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.804113	2.989927	0.134115
2	6	0	3.615402	2.231106	0.066708
3	6	0	2.369748	2.910129	0.083842
4	6	0	2.375521	4.320961	0.162021
5	6	0	3.562488	5.030926	0.218409
6	6	0	4.809586	4.378042	0.206872
7	6	0	1.127782	2.134643	0.023954
8	6	0	1.149929	0.711770	0.021341
9	6	0	-0.059983	-0.001679	-0.051862
10	6	0	-1.301627	0.636531	-0.109976
11	6	0	-1.321159	2.045545	-0.092550
12	6	0	-0.138082	2.755615	-0.035199
13	5	0	3.644793	0.685027	0.027157
14	7	0	2.379820	0.012829	0.060055
15	6	0	5.006102	-0.115286	-0.073763
16	6	0	2.318649	-1.435229	0.112633
17	6	0	5.843551	0.096167	-1.188141
18	6	0	7.064096	-0.567474	-1.328421
19	6	0	7.495159	-1.450288	-0.337652
20	6	0	6.693908	-1.665251	0.785038
21	6	0	5.466954	-1.011949	0.907811
22	6	0	2.414642	-2.179555	-1.075407
23	6	0	2.366321	-3.575139	-0.990375
24	6	0	2.224579	-4.239649	0.230331
25	6	0	2.110155	-3.467381	1.390014
26	6	0	2.149802	-2.070081	1.356854
27	6	0	2.561204	-1.504354	-2.417913
28	6	0	1.990862	-1.275643	2.632455
29	6	0	2.212739	-5.749149	0.297210
30	6	0	-2.552816	-0.121194	-0.201280
31	16	0	-2.682090	-1.778552	0.359517
32	6	0	-4.360788	-1.887922	-0.119635
33	6	0	-4.793935	-0.705367	-0.675770
34	6	0	-3.761159	0.284746	-0.712854

35	6	0	6.095315	5.166844	0.277104
36	6	0	-5.121606	-3.158046	0.127827
37	1	0	5.754207	2.462662	0.135432
38	1	0	1.445457	4.878256	0.187532
39	1	0	3.528366	6.117210	0.279933
40	1	0	-0.023595	-1.083392	-0.092717
41	1	0	-2.267846	2.576155	-0.106774
42	1	0	-0.196975	3.837954	-0.032296
43	1	0	5.534310	0.796297	-1.961704
44	1	0	7.679920	-0.388914	-2.206627
45	1	0	8.448048	-1.964013	-0.437483
46	1	0	7.022708	-2.346852	1.565829
47	1	0	4.860829	-1.205307	1.788150
48	1	0	2.438699	-4.156304	-1.907566
49	1	0	1.981950	-3.963836	2.349912
50	1	0	1.831768	-0.697579	-2.547354
51	1	0	3.558644	-1.063708	-2.533624
52	1	0	2.418905	-2.224961	-3.229031
53	1	0	1.947657	-1.941846	3.499239
54	1	0	2.817745	-0.572793	2.785882
55	1	0	1.070868	-0.679128	2.620218
56	1	0	1.802740	-6.187837	-0.618796
57	1	0	3.227941	-6.149150	0.422533
58	1	0	1.615827	-6.109078	1.142101
59	1	0	-3.910763	1.266489	-1.151618
60	1	0	6.967522	4.505744	0.277750
61	1	0	6.194386	5.850200	-0.576239
62	1	0	6.140621	5.781768	1.185072
63	1	0	-6.067902	-3.152736	-0.421434
64	1	0	-4.556064	-4.040438	-0.193724
65	1	0	-5.359035	-3.292653	1.191380
66	6	0	-6.192877	-0.434019	-1.177830
67	1	0	-6.135795	0.239011	-2.044186
68	1	0	-6.652229	-1.360185	-1.545999
69	6	0	-7.117735	0.195766	-0.116679
70	1	0	-7.194169	-0.485599	0.742037
71	1	0	-6.652547	1.114622	0.266695
72	6	0	-8.519697	0.511886	-0.652263
73	1	0	-8.970178	-0.406650	-1.057783
74	1	0	-8.435959	1.207293	-1.500853
75	6	0	-9.457589	1.110710	0.403620

76	1	0	-9.548880	0.410280	1.247196
77	1	0	-9.005006	2.024437	0.816964
78	6	0	-10.856620	1.438661	-0.134122
79	1	0	-11.305251	0.527446	-0.555067
80	1	0	-10.765957	2.146152	-0.970659
81	6	0	-11.791606	2.022952	0.929638
82	1	0	-12.780314	2.248532	0.513910
83	1	0	-11.932146	1.321941	1.761685
84	1	0	-11.385734	2.952788	1.346997

Zero-point correction=	0.711456
Thermal correction to Energy=	0.753043
Thermal correction to Enthalpy=	0.753987
Thermal correction to Gibbs Free Energy=	0.630810
Sum of electronic and zero-point Energies=	-1988.659950
Sum of electronic and thermal Energies=	-1988.618364
Sum of electronic and thermal Enthalpies=	-1988.617419
Sum of electronic and thermal Free Energies=	-1988.740596

Table S27 Cartesian coordinates of optimized geometry of **P2-F** (DFT, B3LYP/6-31g*)
Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.800174	-2.778183	-0.825060
2	6	0	3.646580	-2.033774	-0.531775
3	6	0	2.402817	-2.701040	-0.520435
4	6	0	2.371744	-4.083268	-0.815067
5	6	0	3.534061	-4.791536	-1.087224
6	6	0	4.781280	-4.147541	-1.093031
7	6	0	1.165923	-1.935020	-0.264831
8	6	0	1.181229	-0.495991	-0.271735
9	6	0	-0.067565	0.171716	-0.185256
10	6	0	-1.283183	-0.500682	-0.024137
11	6	0	-1.274049	-1.904421	0.055159
12	6	0	-0.065675	-2.577598	-0.066535
13	5	0	3.795051	-0.448741	-0.255139
14	7	0	2.360103	0.208121	-0.352547
15	6	0	4.520776	-0.148314	1.186402
16	6	0	2.298841	1.625736	-0.570969
17	6	0	4.172501	-0.830285	2.367162
18	6	0	4.790353	-0.563637	3.590943
19	6	0	5.796412	0.403503	3.671453
20	6	0	6.174619	1.087667	2.513858
21	6	0	5.546355	0.807459	1.296584
22	6	0	2.215578	2.537193	0.500942
23	6	0	2.201800	3.912377	0.224527
24	6	0	2.264944	4.410919	-1.075553
25	6	0	2.315679	3.488622	-2.125832
26	6	0	2.329306	2.110587	-1.899452
27	6	0	2.114682	2.082592	1.939124
28	6	0	2.364881	1.153164	-3.066154
29	6	0	2.285876	5.898733	-1.344755
30	6	0	-2.550835	0.230411	0.082372
31	16	0	-2.759874	1.831045	-0.613887
32	6	0	-4.417191	1.943700	-0.060141
33	6	0	-4.785940	0.802392	0.613814
34	6	0	-3.722689	-0.155224	0.687170

35	6	0	6.052984	-4.916896	-1.369799
36	6	0	-5.221814	3.173077	-0.368803
37	1	0	5.754079	-2.252387	-0.845974
38	1	0	1.425129	-4.613785	-0.868697
39	1	0	3.473073	-5.855803	-1.314892
40	1	0	-0.068129	1.255522	-0.201882
41	1	0	-2.201051	-2.458726	0.168302
42	1	0	-0.083201	-3.662012	-0.013489
43	1	0	3.397319	-1.594496	2.326109
44	1	0	4.490846	-1.111598	4.483737
45	1	0	6.282796	0.615650	4.622380
46	1	0	6.963201	1.838440	2.560164
47	1	0	5.851853	1.338337	0.398408
48	1	0	2.132870	4.609635	1.059180
49	1	0	2.342053	3.851079	-3.153182
50	1	0	1.596944	1.124735	2.023799
51	1	0	3.105356	1.951950	2.387016
52	1	0	1.569591	2.825707	2.533891
53	1	0	2.331308	1.698051	-4.016868
54	1	0	3.275757	0.550750	-3.025701
55	1	0	1.515579	0.460443	-3.038430
56	1	0	1.890168	6.464918	-0.493673
57	1	0	3.306361	6.263070	-1.530950
58	1	0	1.688384	6.157930	-2.227634
59	1	0	-3.818189	-1.097966	1.217127
60	1	0	6.873530	-4.241982	-1.637879
61	1	0	6.381148	-5.494221	-0.492840
62	1	0	5.924554	-5.633603	-2.191806
63	1	0	-6.157617	3.177146	0.199802
64	1	0	-4.676936	4.090758	-0.114120
65	1	0	-5.485240	3.239885	-1.433602
66	6	0	-6.151369	0.533972	1.201871
67	1	0	-6.033762	-0.001295	2.154800
68	1	0	-6.657810	1.477006	1.446127
69	6	0	-7.064041	-0.296228	0.277023
70	1	0	-7.190320	0.239391	-0.674202
71	1	0	-6.558491	-1.239281	0.027649
72	6	0	-8.438885	-0.593861	0.888213
73	1	0	-8.939135	0.354210	1.138863
74	1	0	-8.305804	-1.126181	1.842215
75	6	0	-9.351158	-1.419226	-0.028351

76	1	0	-9.480428	-0.890241	-0.984534
77	1	0	-8.854710	-2.369739	-0.274346
78	6	0	-10.730386	-1.711758	0.576499
79	1	0	-11.227354	-0.761702	0.820671
80	1	0	-10.601997	-2.240468	1.531934
81	6	0	-11.633750	-2.537415	-0.345559
82	1	0	-12.611792	-2.726745	0.112663
83	1	0	-11.806184	-2.020187	-1.297720
84	1	0	-11.180461	-3.509316	-0.577027
85	9	0	4.622615	0.143969	-1.275073

Zero-point correction=	0.711132
Thermal correction to Energy=	0.753981
Thermal correction to Enthalpy=	0.754926
Thermal correction to Gibbs Free Energy=	0.629274
Sum of electronic and zero-point Energies=	-2088.587290
Sum of electronic and thermal Energies=	-2088.544440
Sum of electronic and thermal Enthalpies=	-2088.543496
Sum of electronic and thermal Free Energies=	-2088.669148

Table S28 Cartesian coordinates of optimized geometry of **P2-F'** (DFT, B3LYP/6-31g*) Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.567201	3.021168	-0.042252
2	6	0	-3.413365	2.247677	0.152012
3	6	0	-2.168049	2.821290	-0.199591
4	6	0	-2.135622	4.116773	-0.755843
5	6	0	-3.300346	4.855381	-0.925981
6	6	0	-4.543447	4.320117	-0.559655
7	6	0	-0.936924	2.030664	-0.024970
8	6	0	-1.009046	0.603201	0.087929
9	6	0	0.204286	-0.122289	0.113375
10	6	0	1.457519	0.500380	0.088893
11	6	0	1.514104	1.905130	0.035610
12	6	0	0.331663	2.630898	-0.017446
13	5	0	-3.443249	0.762792	0.813785
14	7	0	-2.236209	-0.032654	0.178602
15	6	0	-4.872482	-0.000705	0.603662
16	6	0	-2.284242	-1.424310	-0.133490
17	6	0	-5.688149	-0.273571	1.716785
18	6	0	-6.943344	-0.877012	1.593494
19	6	0	-7.430509	-1.227533	0.333455
20	6	0	-6.649339	-0.960013	-0.793773
21	6	0	-5.398667	-0.355073	-0.652649
22	6	0	-2.426394	-2.410093	0.866526
23	6	0	-2.493184	-3.758790	0.488688
24	6	0	-2.421232	-4.168130	-0.841523
25	6	0	-2.260071	-3.178999	-1.817263
26	6	0	-2.187926	-1.824074	-1.490813
27	6	0	-2.495090	-2.062753	2.334644
28	6	0	-2.001707	-0.802003	-2.586900
29	6	0	-2.533611	-5.627170	-1.221957
30	6	0	2.699385	-0.278251	0.156269
31	16	0	2.804150	-1.915212	-0.475589
32	6	0	4.485448	-2.072684	-0.010115
33	6	0	4.936042	-0.919922	0.590357
34	6	0	3.917454	0.084632	0.676562

35	6	0	-5.812617	5.128631	-0.708737
36	6	0	5.219943	-3.348725	-0.304232
37	1	0	-5.529614	2.586091	0.222803
38	1	0	-1.194311	4.543557	-1.093296
39	1	0	-3.247353	5.852134	-1.363941
40	1	0	0.152418	-1.201198	0.214891
41	1	0	2.472786	2.415036	0.004557
42	1	0	0.393384	3.714993	-0.057222
43	1	0	-5.316776	0.003042	2.700202
44	1	0	-7.542842	-1.072730	2.482118
45	1	0	-8.406528	-1.698941	0.228996
46	1	0	-7.016673	-1.223864	-1.784784
47	1	0	-4.816377	-0.149059	-1.548611
48	1	0	-2.597647	-4.511192	1.270321
49	1	0	-2.194132	-3.469603	-2.865648
50	1	0	-2.036072	-1.096726	2.546729
51	1	0	-3.537532	-1.983891	2.666772
52	1	0	-2.010977	-2.843615	2.934548
53	1	0	-2.214936	-1.240808	-3.568300
54	1	0	-2.652273	0.065080	-2.436615
55	1	0	-0.973917	-0.417257	-2.605932
56	1	0	-2.310198	-6.280218	-0.370383
57	1	0	-3.546194	-5.880237	-1.567673
58	1	0	-1.844045	-5.888062	-2.034542
59	1	0	4.077369	1.044331	1.158493
60	1	0	-6.691873	4.478661	-0.782766
61	1	0	-5.975969	5.794918	0.151370
62	1	0	-5.786348	5.764364	-1.603303
63	1	0	6.189114	-3.364719	0.204823
64	1	0	4.656788	-4.228955	0.030368
65	1	0	5.411955	-3.478132	-1.378449
66	6	0	6.337303	-0.685720	1.103913
67	1	0	6.283088	-0.156145	2.066017
68	1	0	6.835347	-1.641160	1.313780
69	6	0	7.218354	0.133637	0.139679
70	1	0	7.286419	-0.395862	-0.820922
71	1	0	6.720909	1.089084	-0.076598
72	6	0	8.627175	0.397914	0.685334
73	1	0	9.121008	-0.562421	0.899286
74	1	0	8.550815	0.919461	1.651474
75	6	0	9.509696	1.219140	-0.263398

76	1	0	9.583829	0.701213	-1.231459
77	1	0	9.019901	2.181719	-0.473073
78	6	0	10.921025	1.478370	0.279375
79	1	0	11.411444	0.516220	0.486633
80	1	0	10.847328	1.995022	1.247124
81	6	0	11.795163	2.301633	-0.672490
82	1	0	12.796493	2.467757	-0.257624
83	1	0	11.914356	1.795236	-1.638537
84	1	0	11.348849	3.284301	-0.869474
85	9	0	-3.204409	0.901966	2.233026

Zero-point correction=	0.711429
Thermal correction to Energy=	0.754079
Thermal correction to Enthalpy=	0.755023
Thermal correction to Gibbs Free Energy=	0.630832
Sum of electronic and zero-point Energies=	-2088.586483
Sum of electronic and thermal Energies=	-2088.543833
Sum of electronic and thermal Enthalpies=	-2088.542889
Sum of electronic and thermal Free Energies=	-2088.667080

Reference

1 N. I. Abdo, A. A. El-Shehawy, A. A. El-Barbary and J.-S. Lee, *Eur. J. Org. Chem.*, 2012, 5540-5551.

2 H. Wang, J. Yang, J. Sun, Y. Xu, Y. Wu, Q. Dong, W.-Y. Wong, Y. Hao, X. Zhang and H. Li, *Macromol. Chem. Phys.*, 2014, **215**, 1060-1067.

3 M. T. Berry, D. Castrejon and J. E. Hein, *Org. Lett.*, 2014, **16**, 3676-3679.

4 G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr., J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision B.01; Gaussian, Inc., Wallingford, CT, **2010**.

5 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.

6 P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627.

7 C. T. Lee, W. T. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.

8 R. Bauernschmitt and R. Ahlrichs, *Chem. Phys. Lett.*, 1996, **256**, 454-464.

9 M. E. Casida, C. Jamorski, K. C. Casida and D. R. Salahub, *J. Chem. Phys.*, 1998, **108**, 4439-4449.

10 G. Sheldrick, *Acta Crystallogr. A*, 2008, **64**, 112-122.

11 X.-Y. Wang, H.-R. Lin, T. Lei, D.-C. Yang, F.-D. Zhuang, J.-Y. Wang, S.-C. Yuan and J. Pei, *Angew. Chem. Int. Ed.*, 2013, **52**, 3117-3120.

12 T. Hatakeyama, S. Hashimoto, S. Seki and M. Nakamura, *J. Am. Chem. Soc.*, 2011, **133**, 18614-18617.

13 S. Yruegas, J. J. Martinez and C. D. Martin, *Chem. Commun.*, 2018, DOI: 10.1039/C8CC01529E.

14 K. Huang and C. D. Martin, *Inorg. Chem.*, 2015, **54**, 1869-1875.

15 H. Braunschweig, M. A. Celik, F. Hupp, I. Krummenacher and L. Mailaender, *Angew. Chem. Int. Ed.*, 2015, **54**, 6347-6351.

16 T. Taniguchi, J. Wang, S. Irle and S. Yamaguchi, *Dalton. Trans.*, 2013, **42**, 620-624.

17 M. J. D. Bosdet, C. A. Jaska, W. E. Piers, T. S. Sorensen and M. Parvez, *Org. Lett.*, 2007, **9**, 1395-1398.

18 A. Wakamiya, T. Taniguchi and S. Yamaguchi, *Angew. Chem. Int. Ed.*, 2006, **45**, 3170-3173.

19 A. W. Baggett, F. Guo, B. Li, S.-Y. Liu and F. Jäkle, *Angew. Chem. Int. Ed.*, 2015, **54**, 11191-11195.

20 J. F. Araneda, W. E. Piers, B. Heyne, M. Parvez and R. McDonald, *Angew. Chem. Int. Ed.*, 2011, **50**, 12214-12217.

21 A. J. V. Marwitz, A. N. Lamm, L. N. Zakharov, M. Vasiliu, D. A. Dixon and S.-Y. Liu, *Chem. Sci.*, 2012, **3**, 825-829.

22 K. D. Harris, B. M. Kariuki, C. Lambropoulos, D. Philp and J. M. Robinson, *Tetrahedron*, 1997, **53**, 8599-8612.

23 E. R. Abbey, L. N. Zakharov and S.-Y. Liu, *J. Am. Chem. Soc.*, 2008, **130**, 7250-7252.
24 M. Schaefer, J. Schaefer, R. D. Dewhurst, W. C. Ewing, M. Krahfuss, M. W. Kuntze-Fechner, M. Wehner, C. Lambert and H. Braunschweig, *Chem.–Eur. J.*, 2016, **22**, 8603-8609.
25 A. Gackstatter, H. Braunschweig, T. Kupfer, C. Voigt and N. Arnold, *Chem.–Eur. J.*, 2016, **22**, 16415-16419.
26 K. Liu, R. A. Lalancette and F. Jäkle, *J. Am. Chem. Soc.*, 2017, **139**, 18170-18173.
27 F. Cheng, E. M. Bonder, A. Doshi and F. Jäkle, *Polym. Chem.*, 2012, **3**, 596-600.
28 Y. Li, Y. Kang, J.-S. Lu, I. Wyman, S.-B. Ko and S. Wang, *Organometallics*, 2014, **33**, 964-973.
29 H. A. Benesi and J. H. Hildebrand, *J. Am. Chem. Soc.*, 1949, **71**, 2703-2707.