Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Sign inversions of circularly polarized luminescence for helical compounds by chemically fine-tuning operations

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Contents

All reactions were carried out under argon using oven-dried glassware. Flash column chromatography was performed on 100-200 mesh silica gel. ^{1}H, and ^{13}C NMR spectra were recorded on Bruker AVIII 300MHz, 400MHz or 500 MHz spectrometers at room temperature. High-resolution mass spectra (HRMS) were measured in the APCI mode. The UV-vis spectra were recorded on PerkinElmer® UV/Vis/NIR spectrometer (Lambda 950), and the fluorescence spectra were recorded on HITACHI® F-7000 Fluorescence Spectrometer at room temperature. CD spectra were obtained on a Jasco-810 spectropolarimeter, and CPL spectra were performed with a JASCO CPL-200 spectrometer or JASCO CPL-300 spectrometer at room temperature. High performance liquid chromatography (HPLC) was performed by Agilent Technologies 1260 infinite at room temperature. Commercial reagents were used without further purification. Anhydrous solvents were dried from 4 Å molecular sieves.

1. Synthesis, resolution and characterization of new compounds

Racemic benzo[5]helicene derivatives **2a-f**[1] and hydro[5]helicene derivatives **3a-d**[2] were prepared according to the previously published methods.

1.1 General method for synthesis and resolution of chiral hydro[5]helicene derivatives 1a-f

To a solution of corresponding diene[1] (2 mmol) in 1,2-dichloroethane (20 mL) was added 2-carboxybenzenediazonium chloride (4 mmol) and propylene oxide (4

mL), and the mixture was refluxed for 6 h. Then, the reaction mixture was concentrated under reduced pressure. After rotatory evaporation and their separation by silica gel column chromatography, a further purification was performed by HPLC to obtain pure chiral products **1a-f**. The conditions and analysis of their purification by HPLC were in the first part of SI. The yields of **1** were calculated according to the sum of enantiomers after HPLC resolution.

P-**1a**: White power (75%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.14 (dd, *J* = 6.5, 3.4 Hz, 2H), 7.52 (dd, *J* = 6.5, 3.3 Hz, 2H), 6.96 (d, *J* = 8.3 Hz, 5H), 6.83 - 6.73 (m, 6H), 6.10 (d, *J* = 7.7 Hz, 2H), 3.60 (s, 6H), 3.37 (d, *J* = 15.9 Hz, 2H), 2.38 (td, *J* = 16.3, 13.7, 2.7 Hz, 4H), 1.50 - 1.44 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 155.4, 140. 6, 136.0, 135.7, 135.1, 131.4, 131.2, 130.7, 130.5, 129.6, 129.5, 128.1, 127.7, 125.8, 124.5, 123.51, 123.50, 123.47, 110.2, 56.3, 29.2, 25.1 ppm. HR MS (APCI): *m/z* 681.2223 $[M + H]^+$; found: 681.2212.

P-**1b**: White power (72%); ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 8.12 (dd, *J* = 6.5, 3.3 Hz, 2H), 7.50 (dd, *J* = 6.5, 3.2 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* = 8.2 Hz, 2H), 6.72 - 6.67 (m, 2H), 6.59 - 6.54 (m, 2H), 6.39 (td, *J* = 8.7, 2.6 Hz, 2H), 6.00 - 5.88 (m, 2H), 3.58 (s, 6H), 3.40 - 3.31 (m, 2H), 2.69 - 2.27 (m, 4H), 1.65 - 1.57 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 126 MHz): δ = 155.4, 135.8, 135.5, 135.2, 133.1, 133.0, 132.7, 132.3, 132.2, 131.7, 130.4, 128.5, 126.9, 125.5, 124.4, 113.5, 113.4, 113.2,

110.1, 56.4, 29.4, 25.0 ppm. HR MS (APCI): *m/z* 581.2287 $[M + H]^+$; found: 581.2288.

P-**1c**: Yellow power (81%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.11 (dd, *J* = 6.5, 3.4 Hz, 2H), 7.48 (dd, *J* = 6.5, 3.3 Hz, 2H), 7.04 - 6.97 (m, 4H), 6.92 (d, *J* = 8.1 Hz, 2H), 6.76 (d, *J* = 8.2 Hz, 2H), 6.70 - 6.60 (m, 4H), 5.96 (d, *J* = 7.6 Hz, 2H), 3.57 (s, 6H), 3.32 - 3.27 (m, 2H), 2.47 - 2.25 (m, 4H), 1.50 - 1.42 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 155.4, 137.0, 135.8, 135.4, 135.2, 132.2, 131.5, 131.0, 130.3, 129.7, 126.6, 125.6, 125.2, 124.3, 110.2, 56.4, 29.4, 25.0 ppm. HR MS (APCI): *m/z* 545.2475 $[M + H]^+$; found: 545.2476.

P-**1d**: White power (75%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.11 (dd, *J* = 6.5, 3.3 Hz, 2H), 7.47 (dd, *J* = 6.5, 3.2 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.80 (d, *J* = 7.4 Hz, 2H), 6.74 (d, *J* = 8.2 Hz, 2H), 6.48 (dd, *J* = 13.3, 7.9 Hz, 4H), 5.84 (d, *J* = 7.3 Hz, 2H), 3.58 (s, 6H), 3.30 (d, *J* = 15.0 Hz, 2H), 2.40 (td, *J* = 15.0, 4.0 Hz, 2H), 2.32 - 2.28 (m, 2H), 2.24 (s, 6H),1.51 - 1.48 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 155.5, 135.9, 135.3, 135.0, 134.9, 133.9, 132.4, 131.1, 130.9, 130.3, 129.5, 127.3, 127.2, 126.4, 125.1, 124.3, 109.9, 56.3, 29.1, 25.0, 21.1 ppm. HR MS (APCI): *m/z* 573.2788 $[M + H]^+$; found: 573.2778.

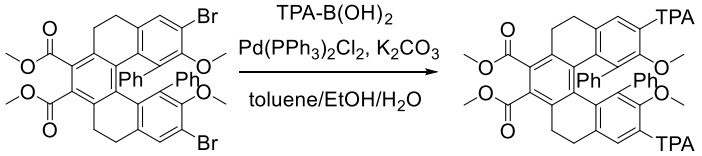
P-**1e**: White power (65%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.12 (dd, *J* = 6.5, 3.4 Hz, 2H), 7.48 (dd, *J* = 6.5, 3.2 Hz, 2H), 6.93 (d, *J* = 7.8 Hz, 2H), 6.74 (d, *J* = 8.1 Hz, 2H), 6.59 - 6.50 (m, 4H), 6.23 (d, *J* = 6.8 Hz, 2H), 5.90 (d, *J* = 8.4 Hz, 2H), 3.73 (s,

6H), 3.58 (s, 6H), 3.33 (dd, *J* = 14.1, 3.3 Hz, 2H), 2.43 - 2.33 (m, 4H), 1.62 (dt, *J* = 13.3, 7.7 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 157.7, 155.6, 135.9, 135.3, 135.1, 132.3, 130.4, 129.6, 129.1, 126.3, 125.1, 124.3, 112.5, 110.0, 100.0, 56.4, 55.2, 31.6, 22.7 ppm. HR MS (APCI): *m/z* 605.2686 $[M + H]^+$; found: 605.2678.

P-**1f**: White power (70%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.13 (dd, *J* = 6.5, 3.4 Hz, 2H), 7.51 (dd, *J* = 6.5, 3.2 Hz, 2H), 6.99 (d, *J* = 8.2 Hz, 2H), 6.97 - 6.92 (m, 2H), 6.76 (d, *J* = 8.2 Hz, 2H), 6.69 - 6.63 (m, 2H), 6.58 - 6.49 (m, 2H), 5.94 - 5.83 (m, 2H), 3.58 (s, 6H), 3.37 (d, *J* = 14.8 Hz, 2H), 2.50 - 2.35 (m, 4H), 1.66 - 1.57 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 13C NMR (126 MHz, CDCl3) δ 155.3, 135.7, 135.6, 135.24, 135.21, 132.6, 132.1, 131.6, 131.5, 130.4, 128.3, 127.2, 126.7, 126.6, 125.6, 124.4, 110.1, 56.3, 29.7, 25.0 ppm. HR MS (APCI): *m/z* 613.1696 $[M + H]^+$; found: 613.1685.

P-**1g**: White power (60%); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.10 (dd, *J* = 6.4, 3.3 Hz, 2H), 7.45 (dd, *J* = 6.5, 3.2 Hz, 2H), 7.22 (d, *J* = 7.5 Hz, 8H), 7.11 (d, *J* = 7.8 Hz, 8H), 7.00 (d, *J* = 7.2 Hz, 4H), 6.96 (d, *J* = 4.2 Hz, 2H), 6.70 (d, *J* = 8.1 Hz, 4H), 6.52 (d, *J* = 7.9 Hz, 2H), 6.37 (d, *J* = 8.3 Hz, 2H), 5.87 (d, *J* = 8.4 Hz, 2H), 3.56 (s, 6H), 3.45 - 3.36 (m, 2H), 2.61 - 2.40 (m, 4H), 1.99 (td, *J* = 14.0, 13.4, 3.5 Hz, 2H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz): δ = 155.7, 147.8, 145.1, 135.6, 135.1, 135.0, 132.2, 132.0, 131.6, 130.8, 130.3, 129.4, 129.0, 126.2, 125.2, 124.6, 124.3, 122.6, 110.9, 56.6, 31.6, 25.2 ppm. HR MS (APCI): *m/z* 879.3945 $[M + H]^+$; found: 879.3965.

1.2 Method for synthesis of chiral 3e:



P- or *M*- **3e**

To a mixture of helically chiral dibromo aromatic esters[2] (0.1 mmol), K_2CO_3 (1 mmol), and arylboronic acid (0.7 mmol) in DMF (20mL) and toluene (10 mL) under argon atmosphere was added catalytic amount of Pd $(PPh_3)_2Cl_2$ (5 mol %), followed by stirring at 120 °C for 12h under argon atmosphere. After cooling, the reaction mixture was poured into ethyl acetate (20 mL). The organic layer was washed with saturated brine (3×20 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The residue was purified by flash column chromatography to afford pure product *P*-**3e** or *M*-**3e**.

P-**3e**: Green solid (63%). ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 7.54 (d, *J* = 8.5 Hz, 4H), 7.29 (d, *J* = 8.0 Hz, 4H), 7.16 (d, *J* = 8.0 Hz, 12H), 7.07 - 7.01 (m, 6H), 6.99 (d, *J* = 6.5 Hz, 2H), 6.95 (s, 2H), 6.85 (dd, *J* = 24.4, 6.6 Hz, 4H), 6.23 (d, *J* = 6.4 Hz, 2H), 3.91 (s, 6H), 2.80 (s, 6H), 2.70 (d, *J* = 16.3 Hz, 2H), 2.46 (td, *J* = 15.2, 3.6 Hz, 2H), 2.22 (d, *J* = 13.2 Hz, 2H), 1.45 - 1.38 (m, 2H) ppm. ^{13}C NMR ($CDCl_3$, 126 MHz): δ = 168.9, 153.8, 147.7, 138.8, 138.2, 136.7, 136.6, 136.5, 134.5, 134.2, 130.6, 130.2, 129.8, 129.31, 129.26, 128.9, 128.6, 127.5, 126.7, 125.9, 124.7, 124.5, 123.19, 123.15, 123.0, 122.9, 59.5, 52.4, 29.6, 27.8 ppm. HR MS (APCI): *m/z* 1097.4485 $[M + H]^+$; found 1097.44835.

References

(1) W.-B. Lin, M. Li, L. Fang, Y. Shen, C.-F. Chen, *Chem. Asian J.* **2017**, *12*, 86-94.

(2) D.-Q. He, H.-Y. Lu, M. Li, C.-F. Chen, *Chem. Commun.* **2017**, *53*, 6093-6096.

1.3 HPLC charts of the enantiomeric resolution

HPLC analysis conditions:

Column: Chiralpak® IE 5 μm, 10 mm × 250 mm

Mobile phase: hexane / dichloromethane

Flow rate: 5 mL/min

Temperature: 20 ℃

Abs. detector: 270 nm

Considering the similar structures of **1** and the same treatment procedure by oxidation, the absolute configuration of **1** was determined by the comparison of retention time in the HPLC charts of the oxidation product of resolved chiral **1a** and those of the enantiomers of **2a** (Fig. S1-S4). Detailed HPLC charts of **1a~f** were then prensented and analyzed (Fig. S5-S25).

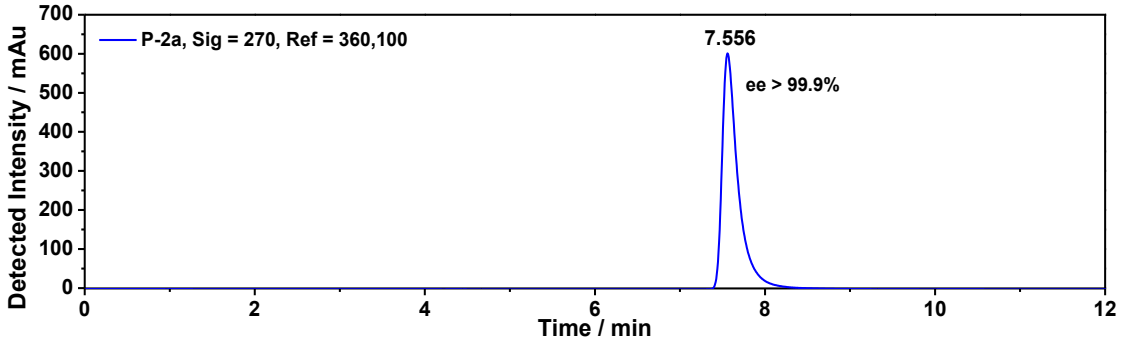


Fig. S1. HPLC profile of resolution of *P*-**2a.**

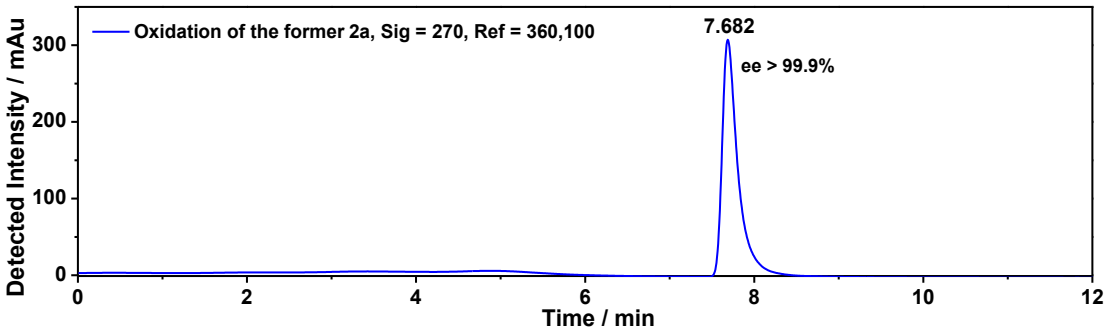


Fig. S2. HPLC profile of the oxidation product of the semi-preparative-resolved **1a** of the former peak.

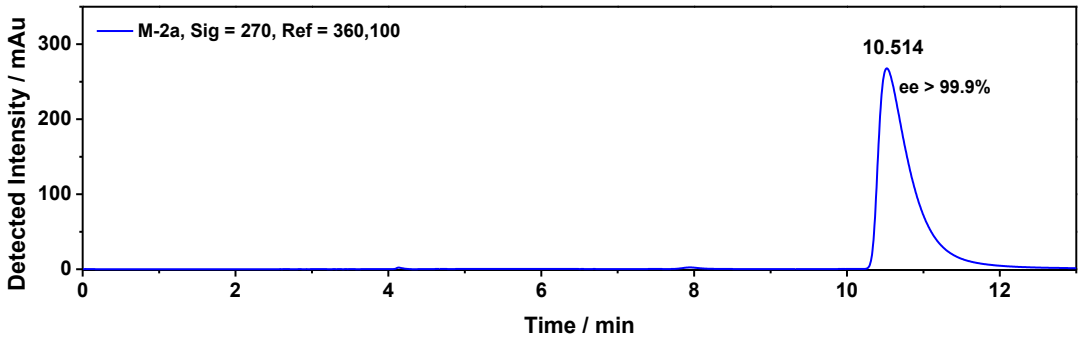


Fig. S3. HPLC profile of resolution of *M*-**2a.**

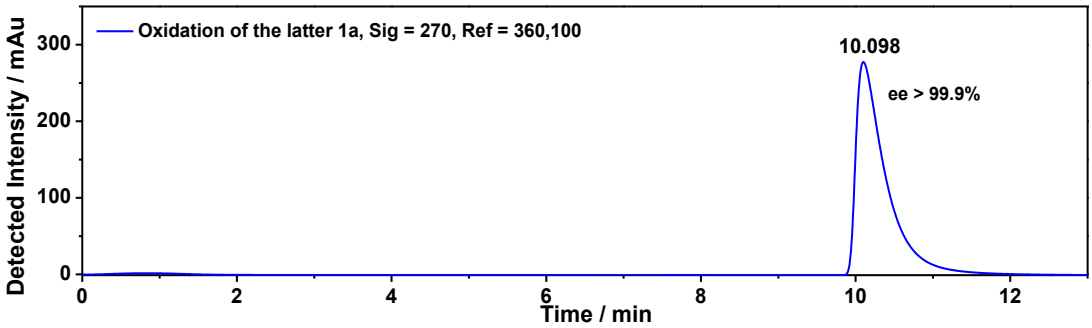


Fig. S4. HPLC profile of the oxidation product of the semi-preparative-resolved **1a** of the latter peak.

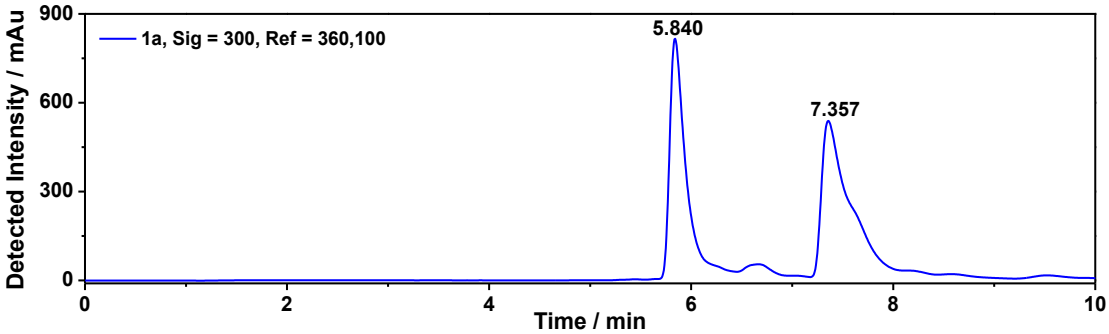


Fig. S5. HPLC profile of resolution of *rac*-**1a.**

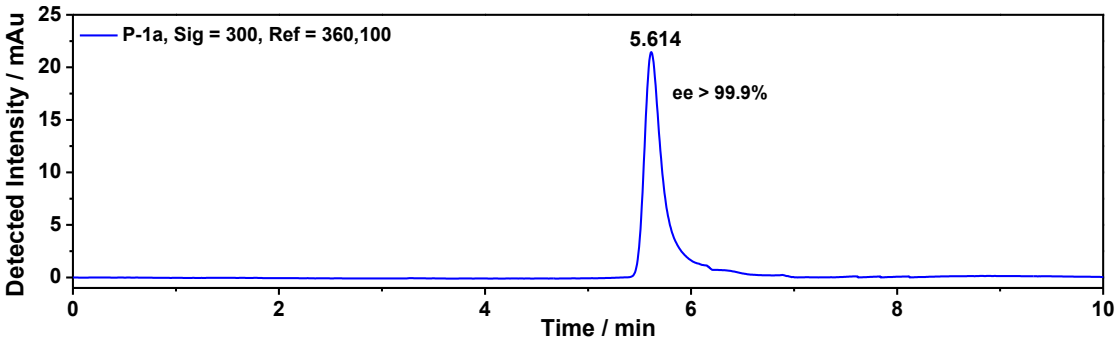


Fig. S6. HPLC profile of *P*-**1a** after resolution**.**

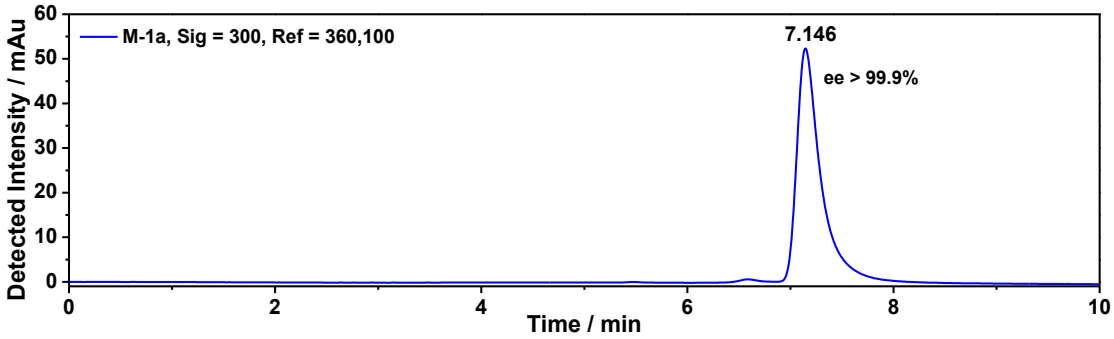


Fig. S7. HPLC profile of *M*-**1a** after resolution**.**

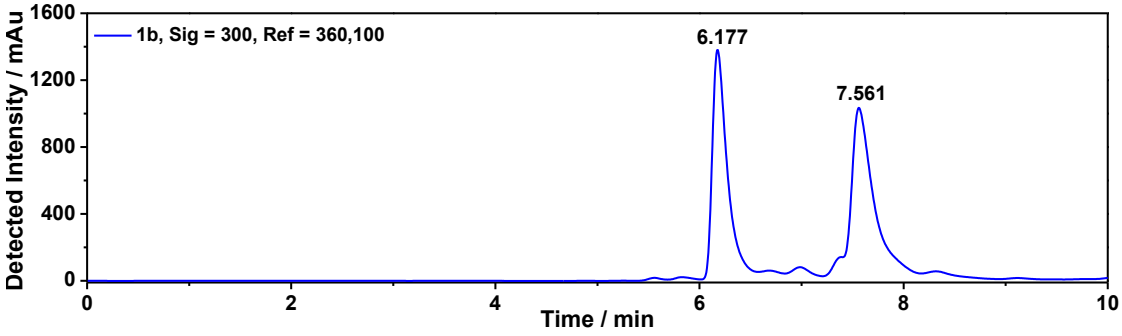


Fig. S8. HPLC profile of resolution of *rac*-**1b.**

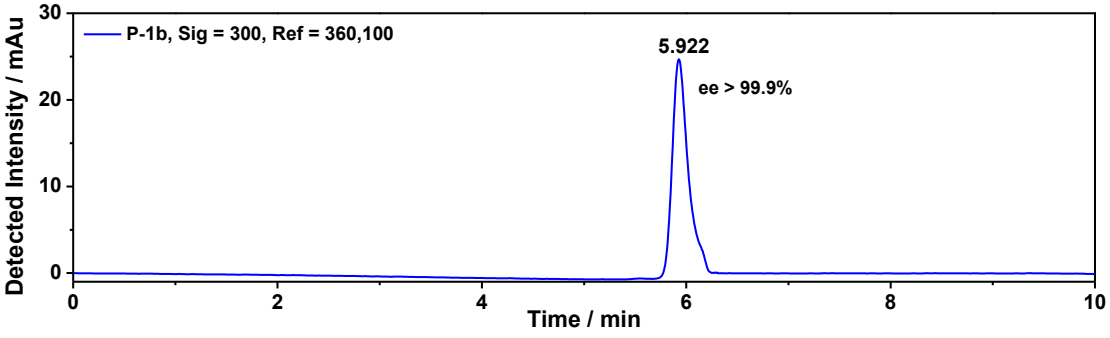


Fig. S9. HPLC profile of *P*-**1b** after resolution**.**

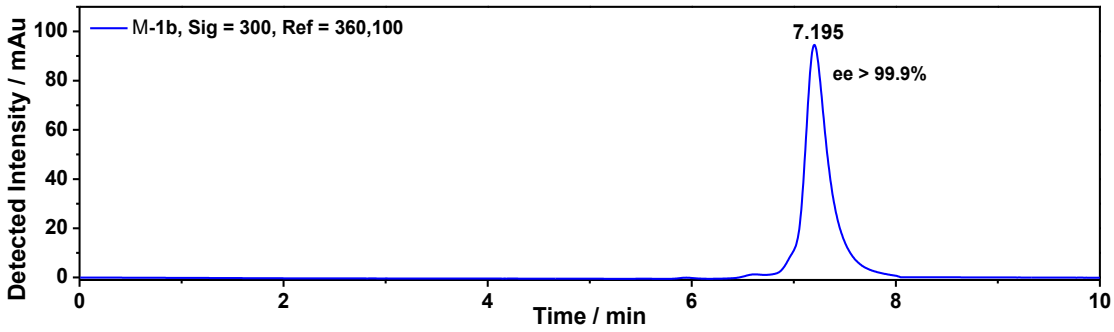


Fig. S10. HPLC profile of *M*-**1b** after resolution**.**

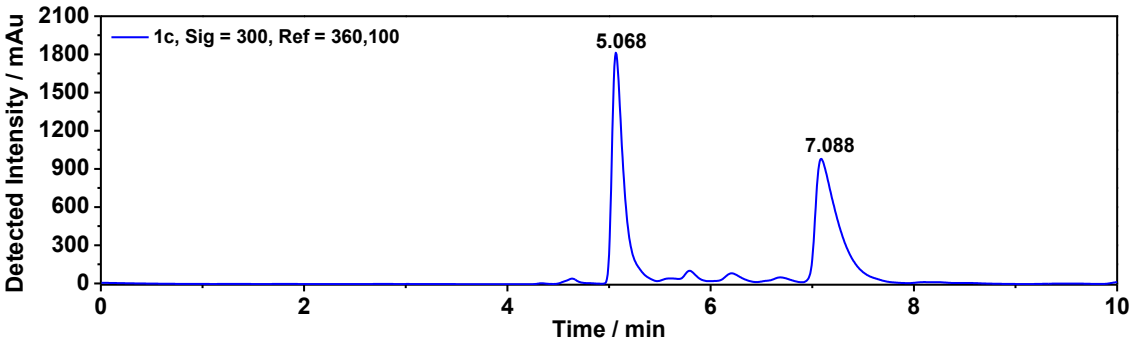


Fig. S11. HPLC profile of resolution of *rac*-**1c.**

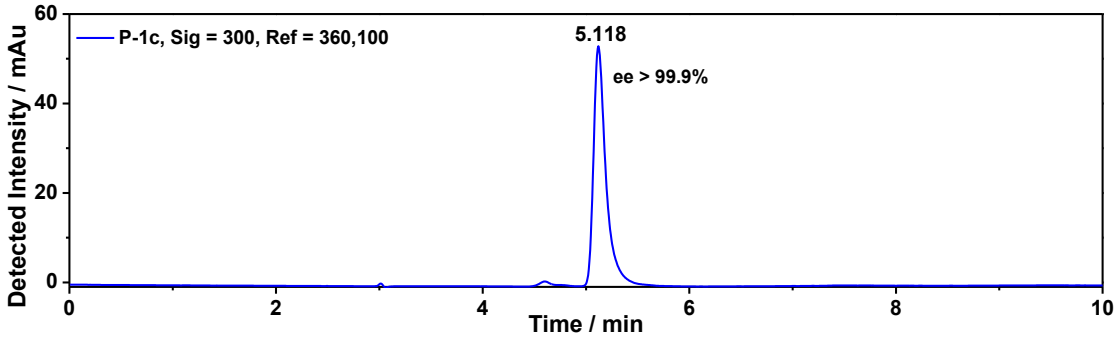


Fig. S12. HPLC profile of *P*-**1c** after resolution**.**

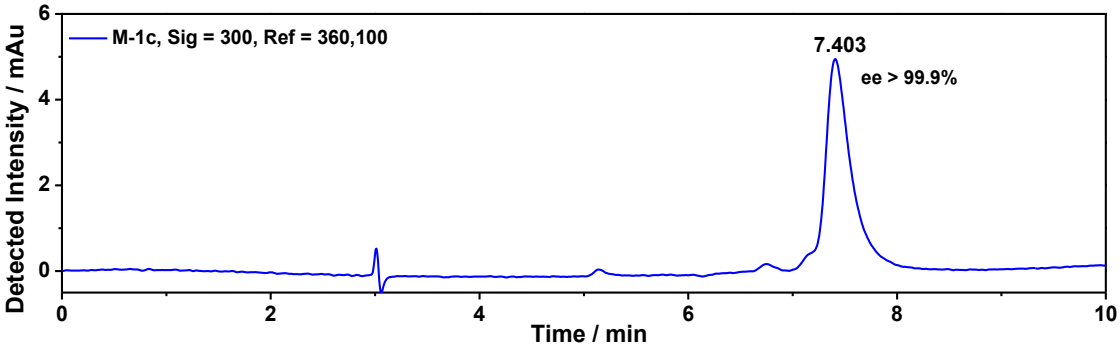


Fig. S13. HPLC profile of *M*-**1c** after resolution**.**

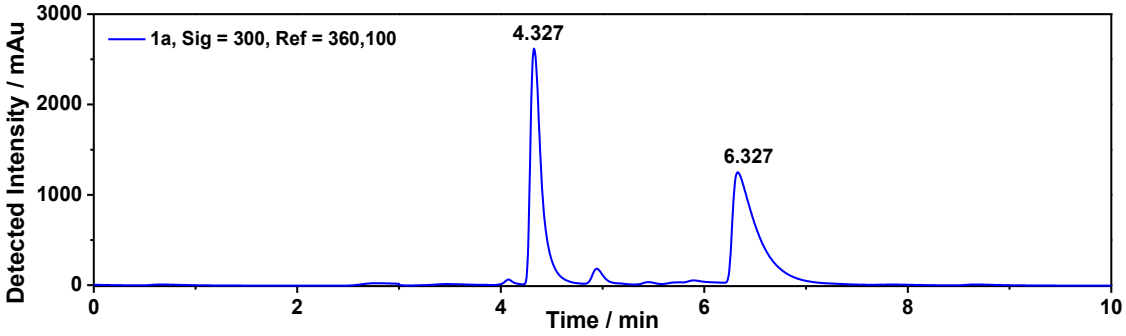


Fig. S14. HPLC profile of resolution of *rac*-**1d.**

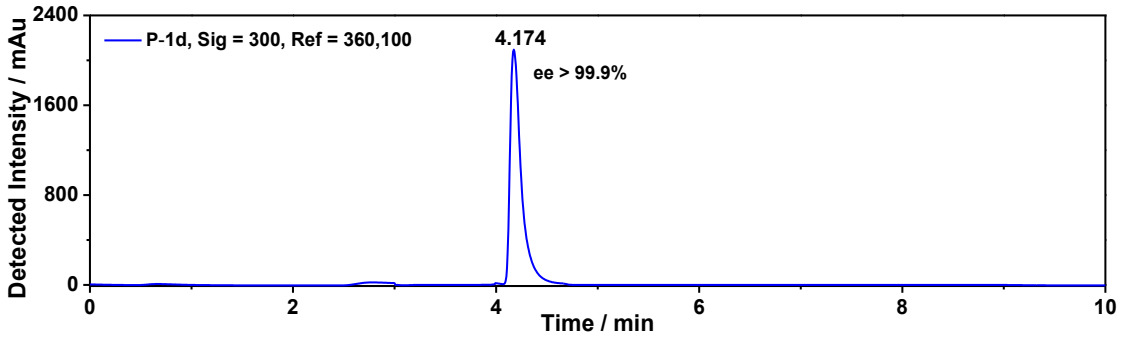


Fig. S15. HPLC profile of *P*-**1d** after resolution**.**

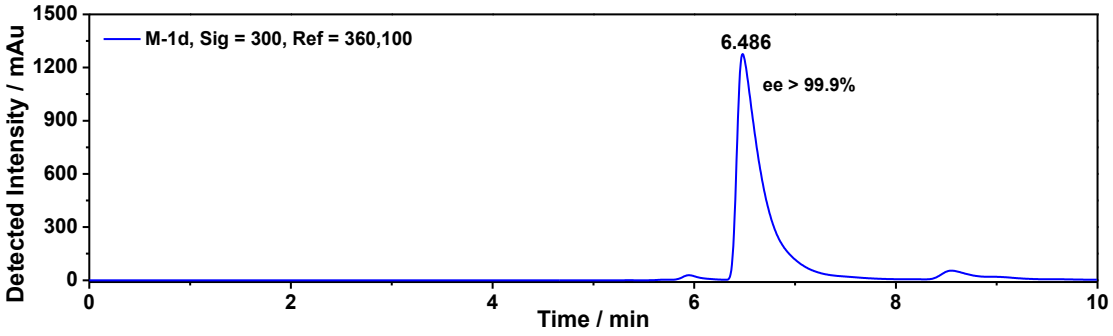


Fig. S16. HPLC profile of *M*-**1d** after resolution**.**

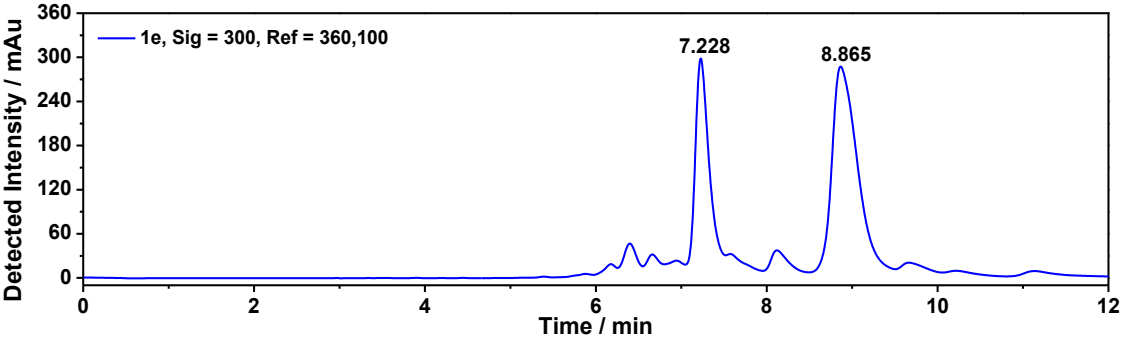


Fig. S17. HPLC profile of resolution of *rac*-**1e.**

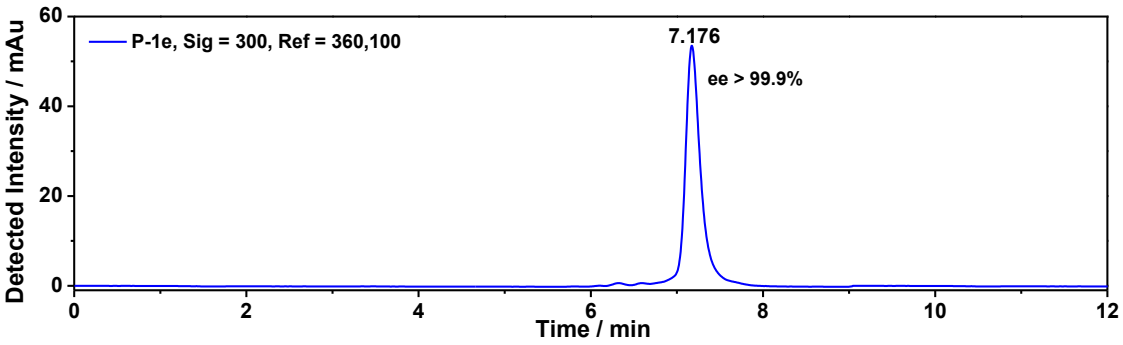


Fig. S18. HPLC profile of *P*-**1e** after resolution**.**

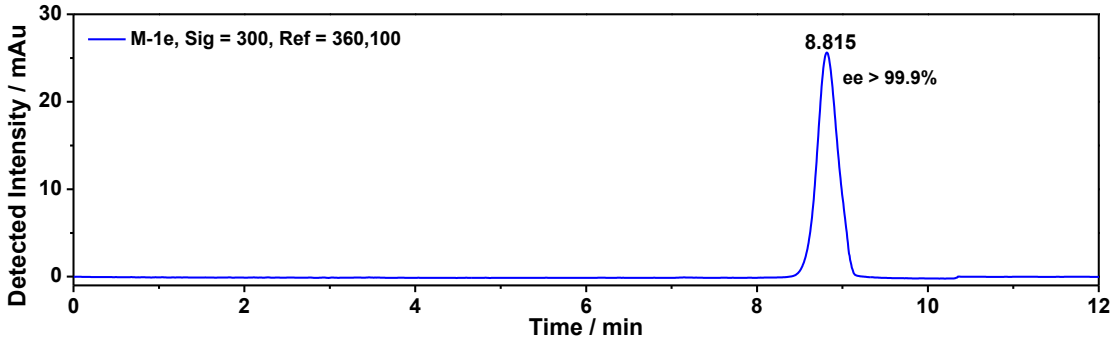


Fig. S19. HPLC profile of *M*-**1e** after resolution**.**

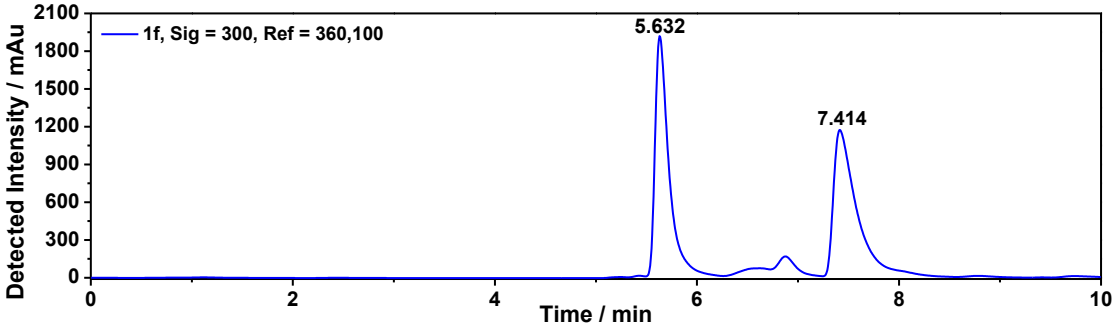


Fig. S20. HPLC profile of resolution of *rac*-**1f.**

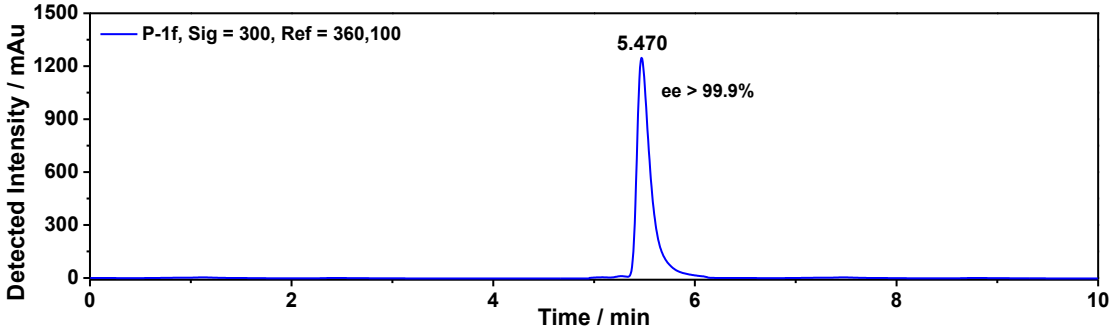


Fig. S21. HPLC profile of *P*-**1f** after resolution**.**

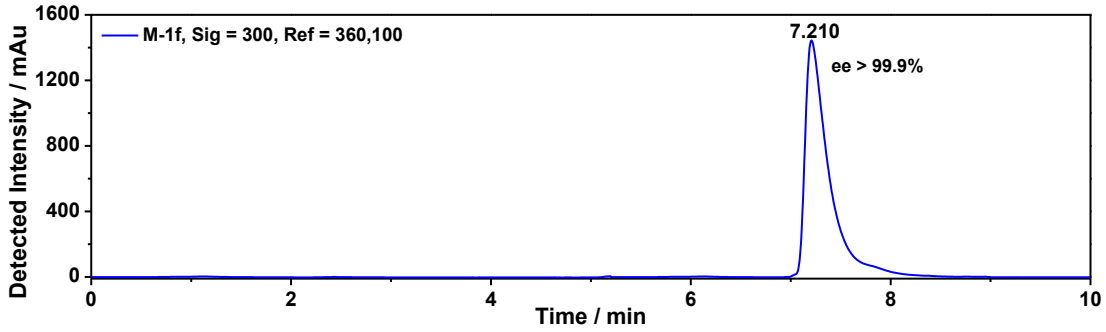


Fig. S22. HPLC profile of *M*-**1f** after resolution**.**

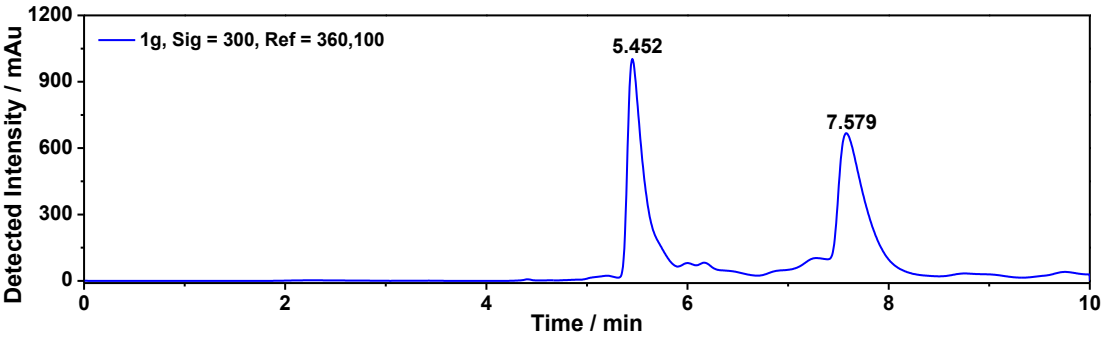


Fig. S23. HPLC profile of resolution of *rac*-**1g.**

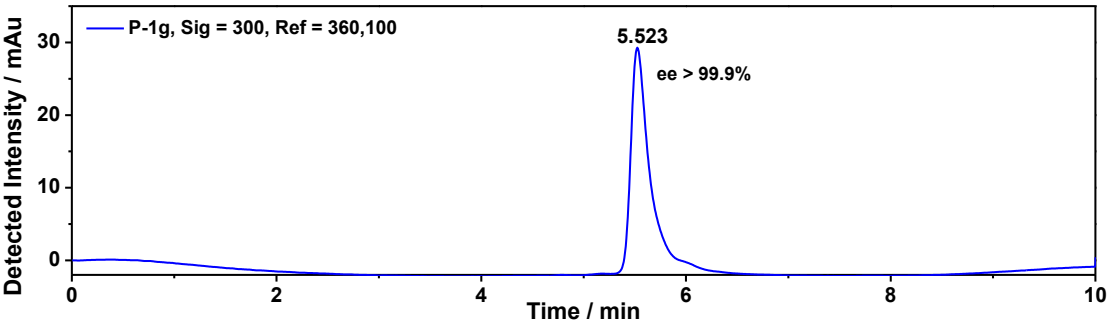


Fig. S24. HPLC profile of *P*-**1g** after resolution**.**

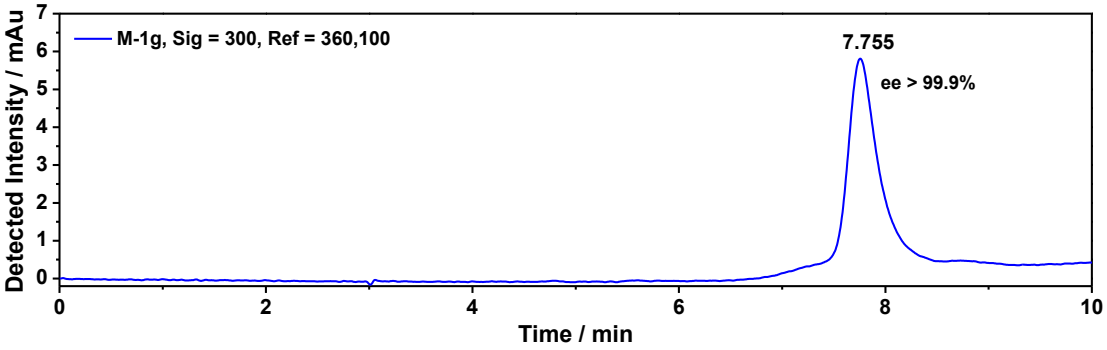


Fig. S25. HPLC profile of *M*-**1g** after resolution**.**

1.4 NMR spectra of new compounds 1a~g and 3e

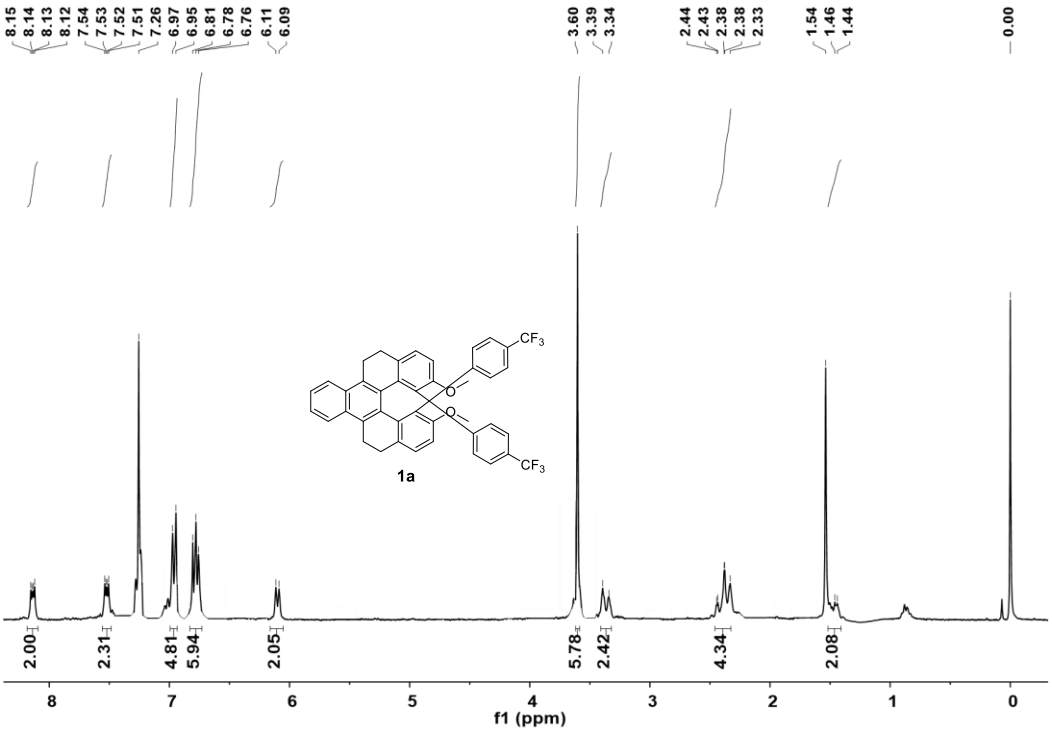


Fig. S26. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of *P*-**1a**.

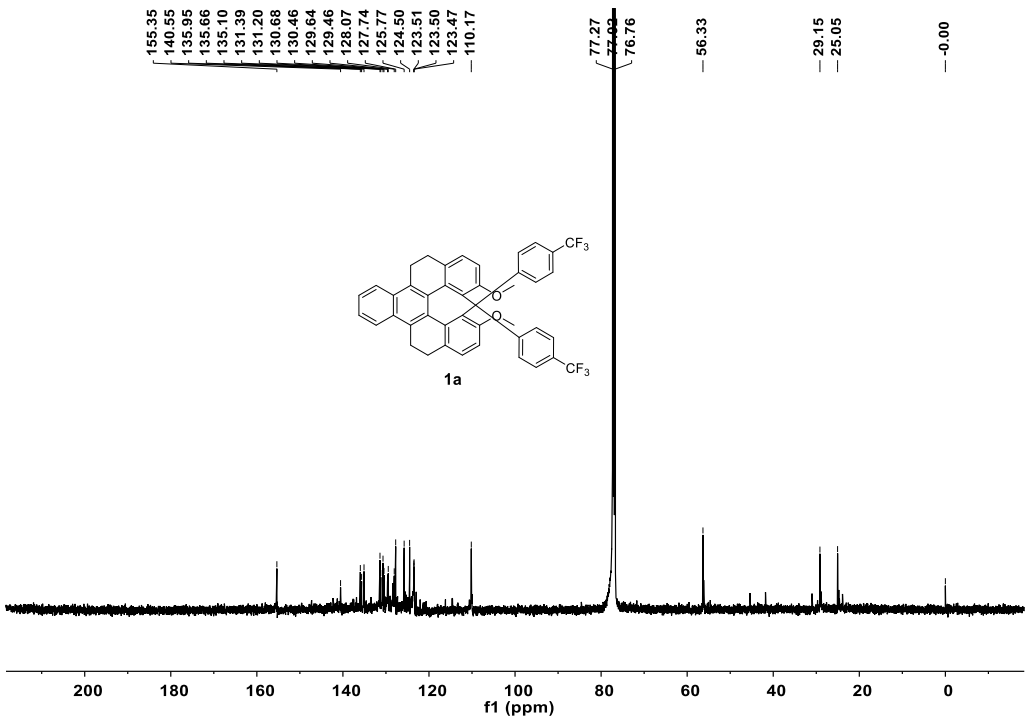


Fig. S27. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of *P*-**1a**.

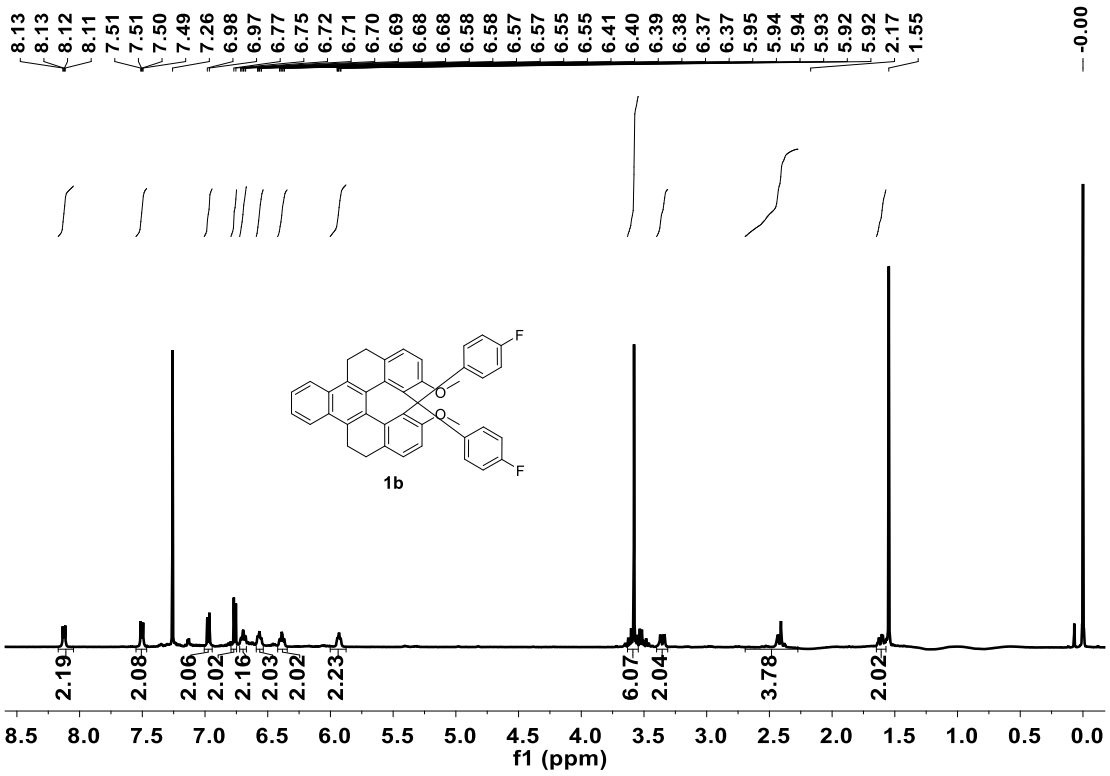


Fig. S28. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of *P*-**1b**.

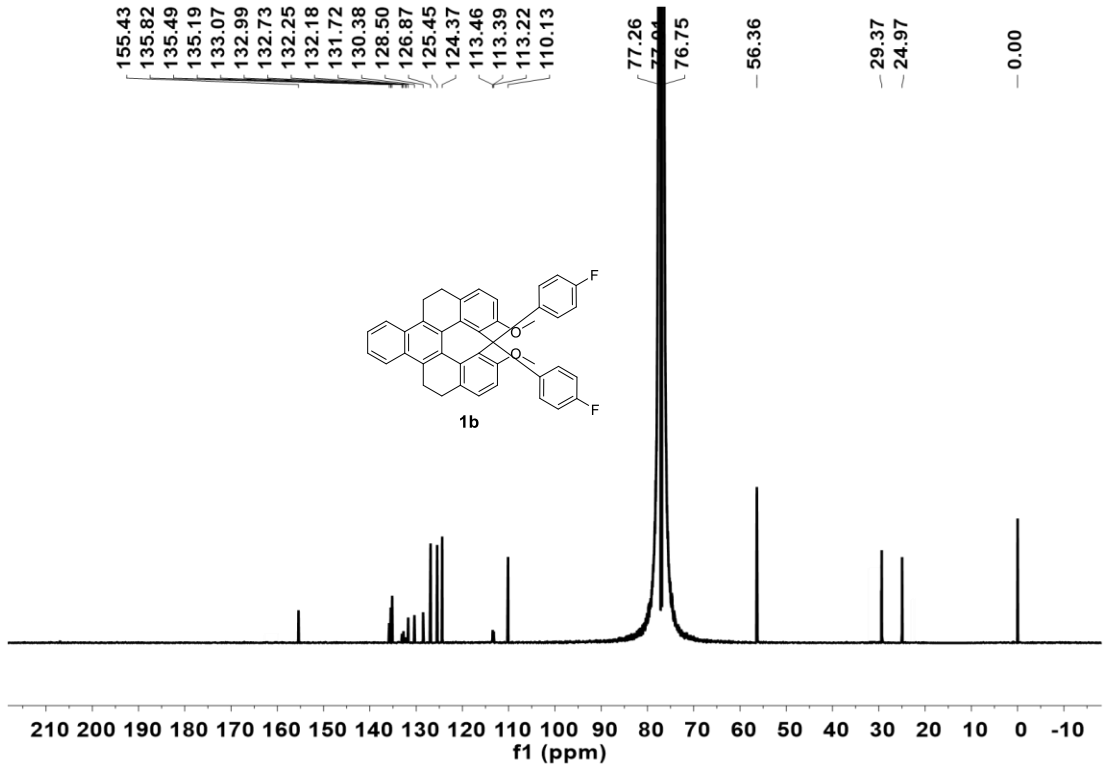


Fig. S29. ^{13}C NMR spectrum (126 MHz, CD_2Cl_2) of *P*-**1b**.

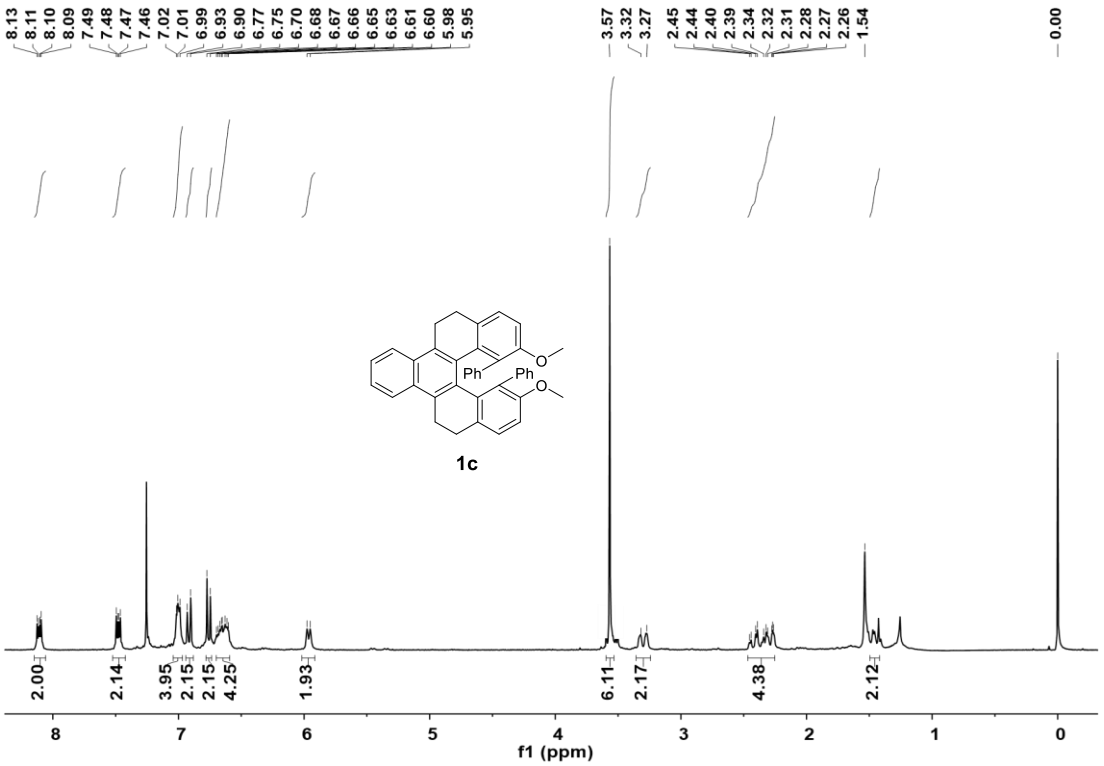


Fig. S30. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of *P*-**1c**.

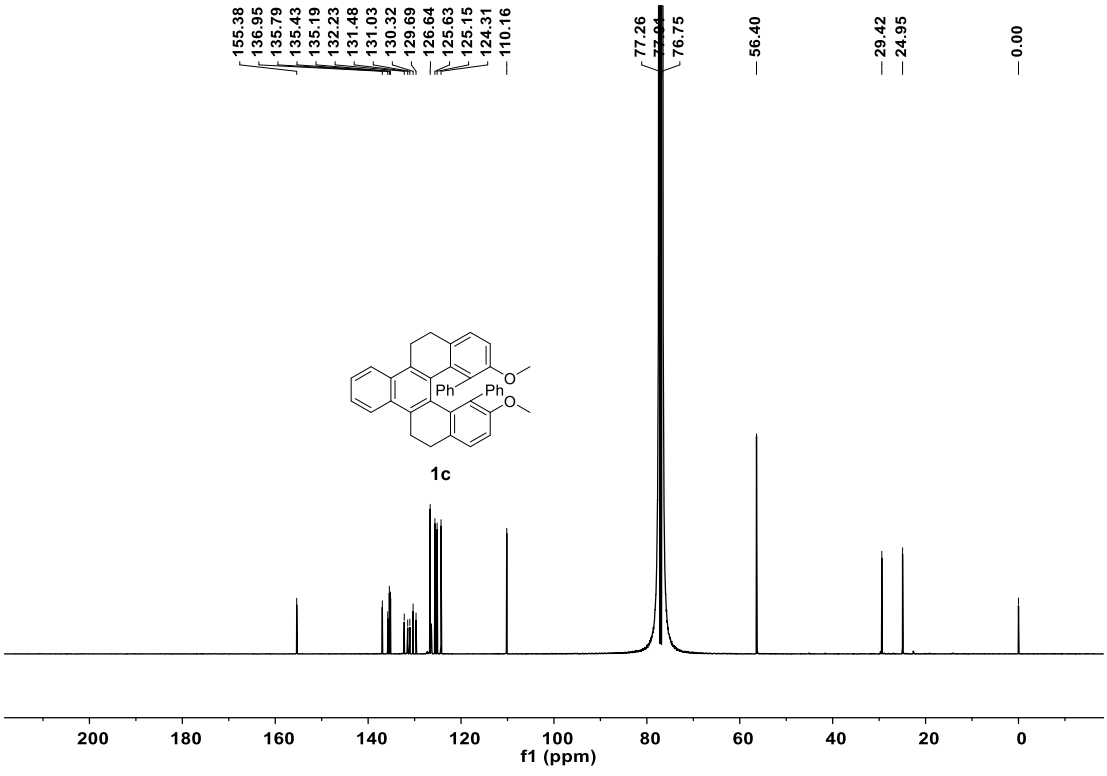


Fig. S31. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of *P*-**1c**.

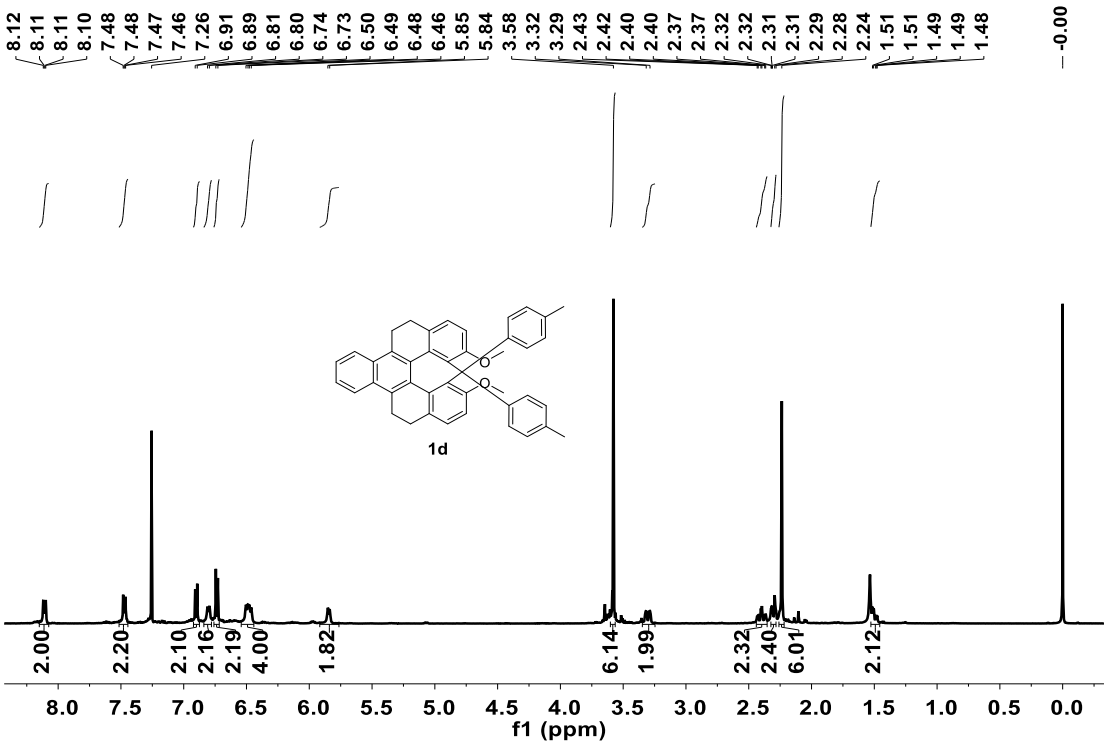


Fig. S32. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of *P*-**1d**.

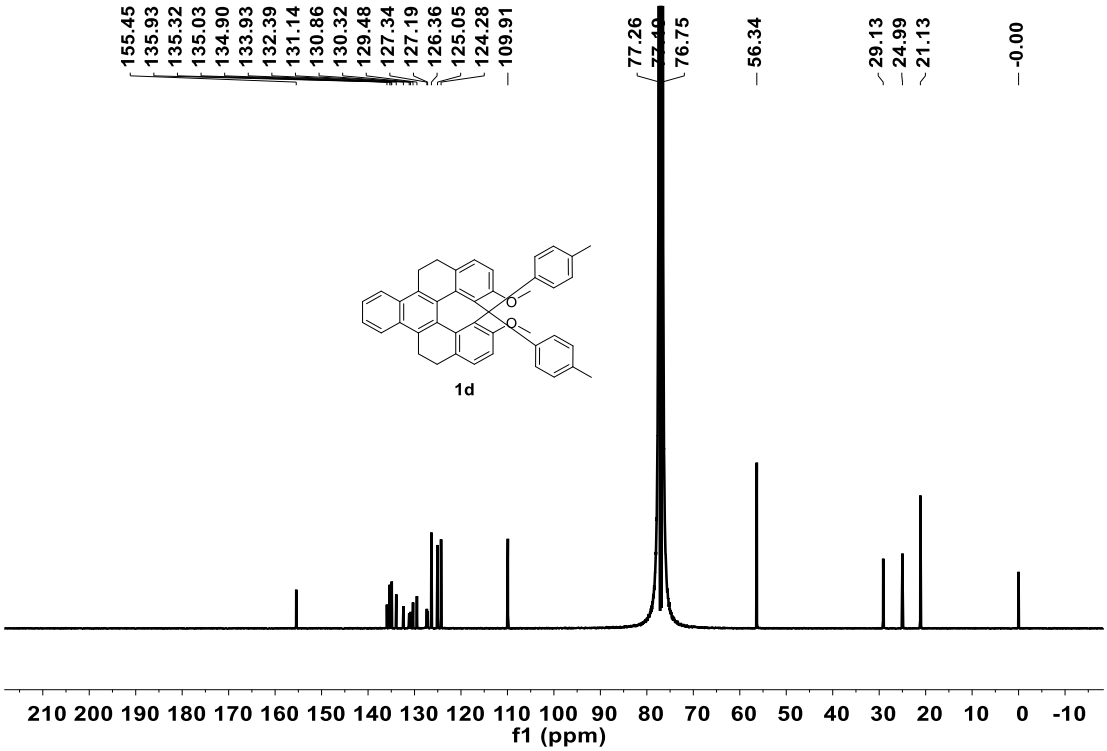


Fig. S33. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of *P*-**1d**.

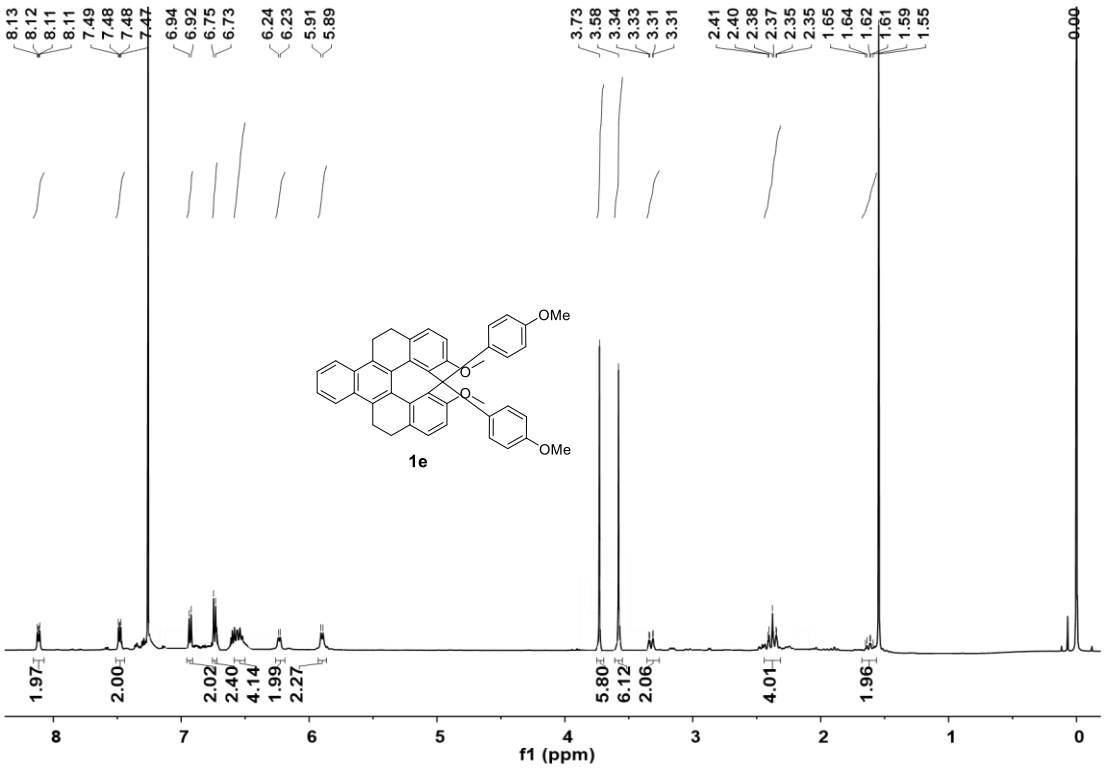


Fig. S34. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of *P*-**1e**.

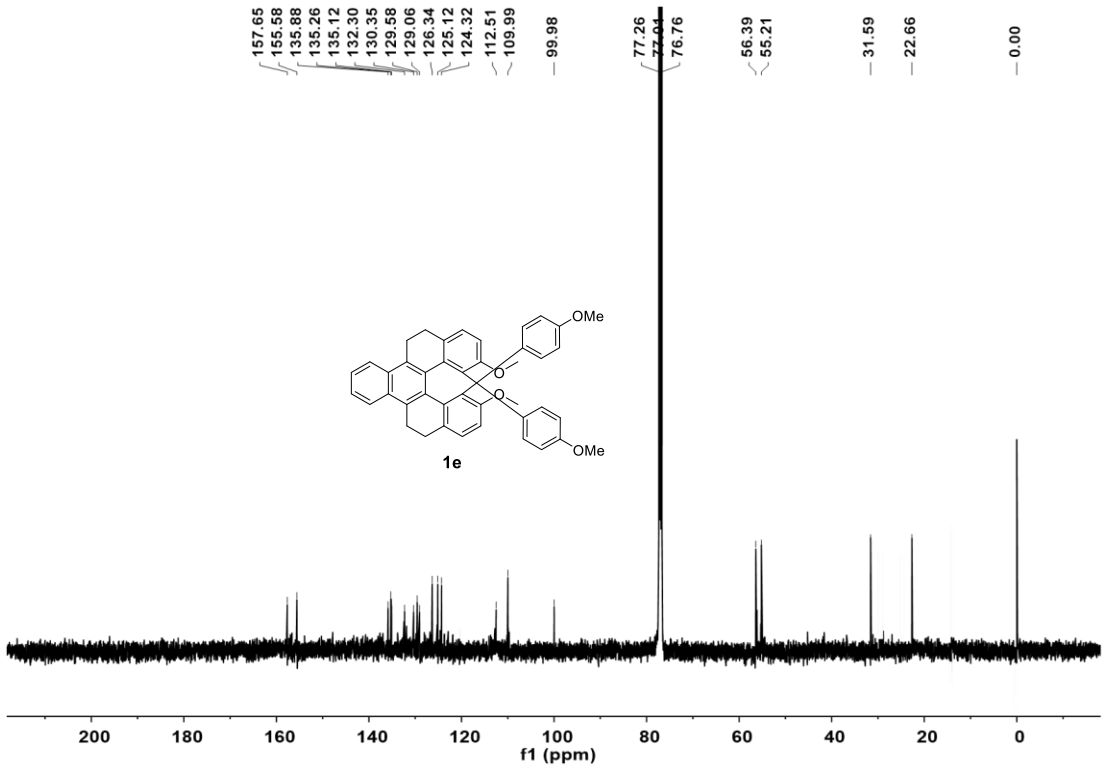


Fig. S35. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of *P*-**1e**.

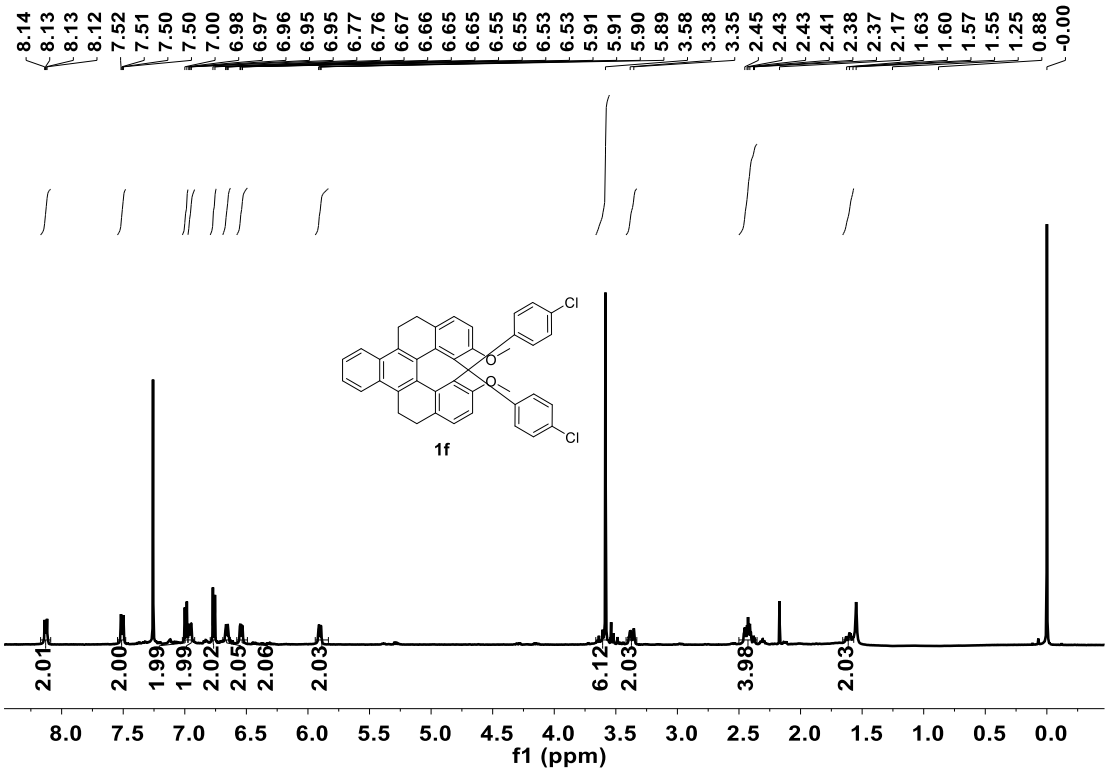


Fig. S36. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of *P*-**1f**.

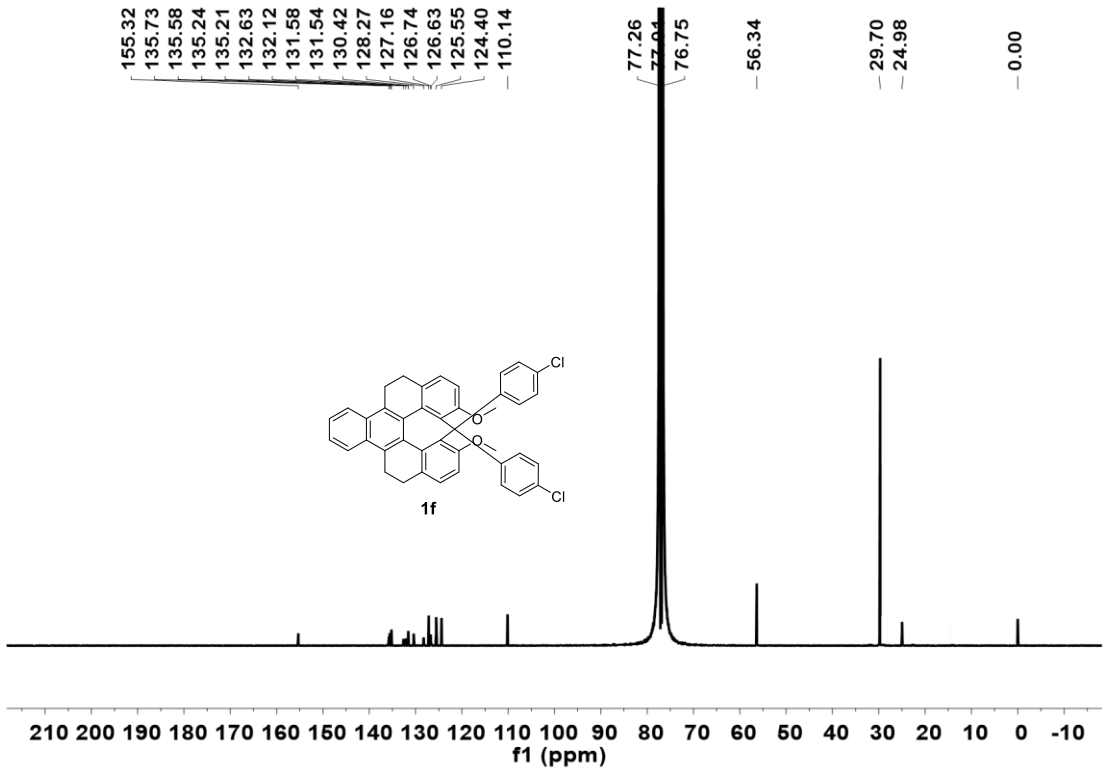


Fig. S37. ^{13}C NMR spectrum (126 MHz, CD_2Cl_2) of *P*-**1f**.

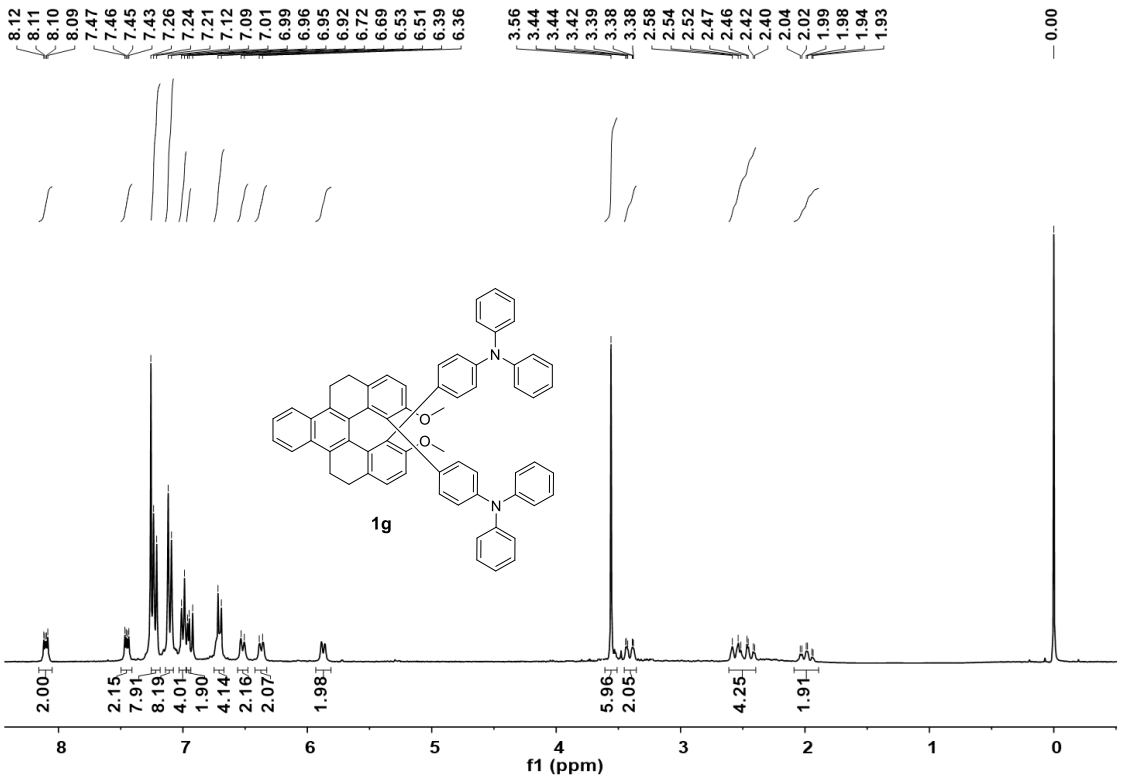


Fig. S38. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of *P*-**1g**.

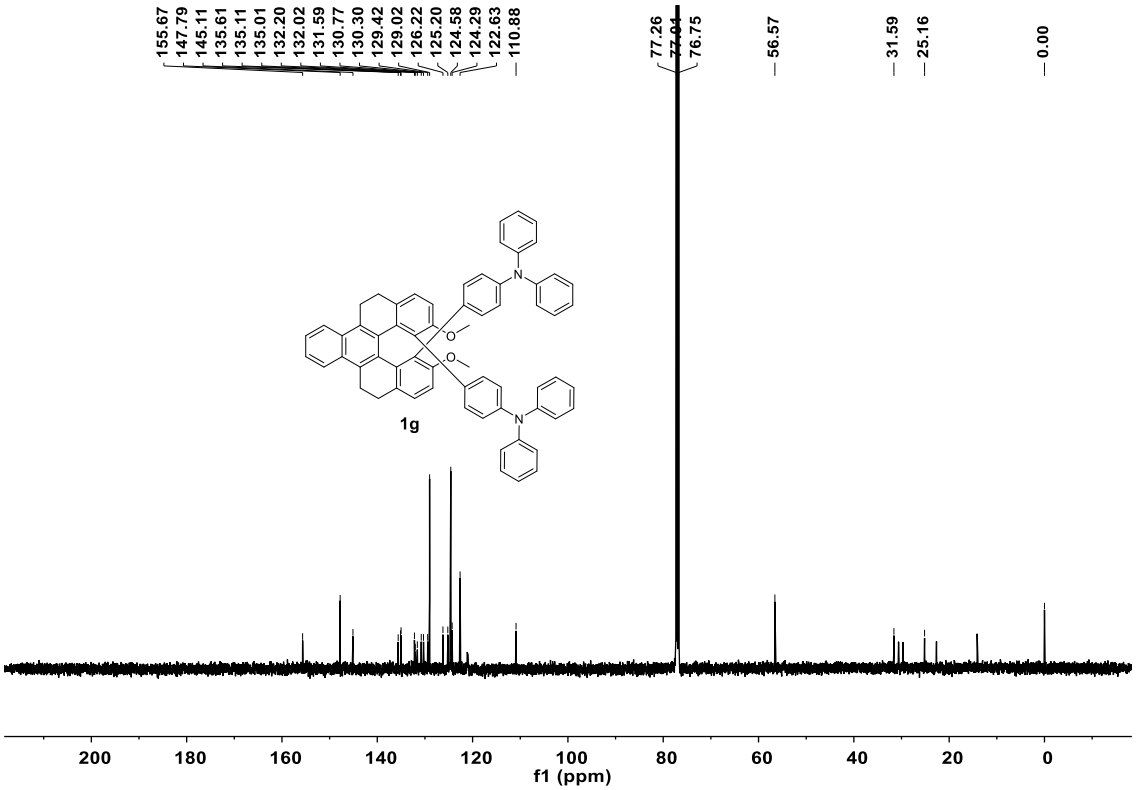


Fig. S39. ^{13}C NMR spectrum (75 MHz, CD_2Cl_2) of *P*-**1g**.

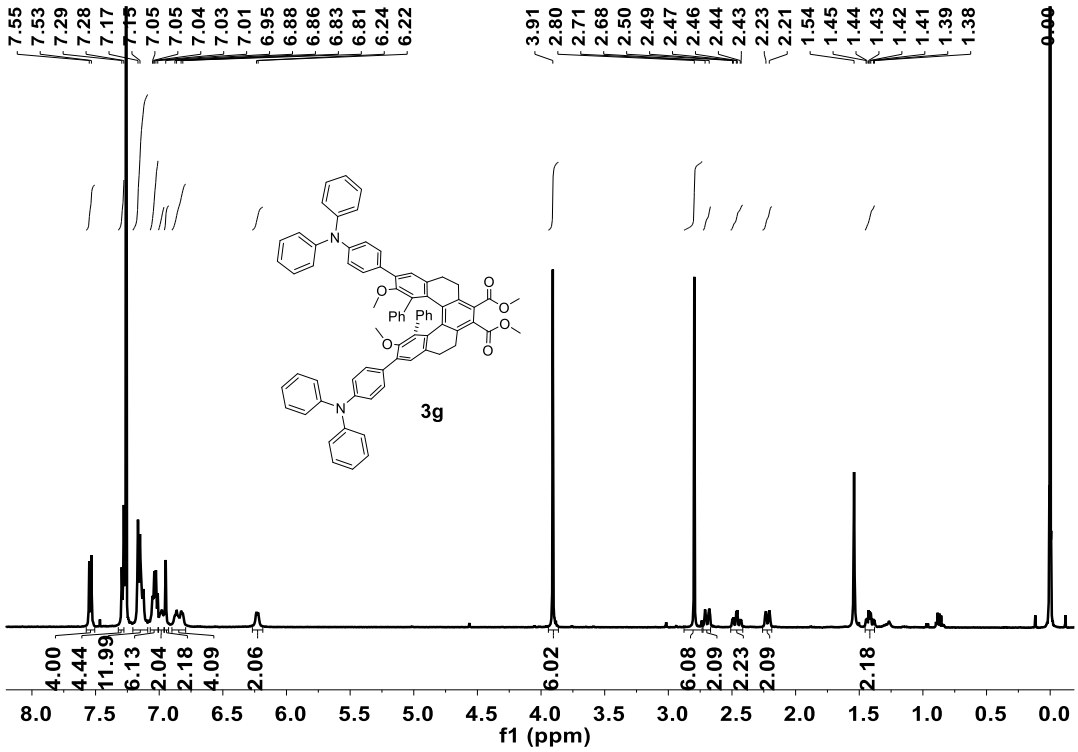


Fig. S40. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2) of *P*-**3g**.

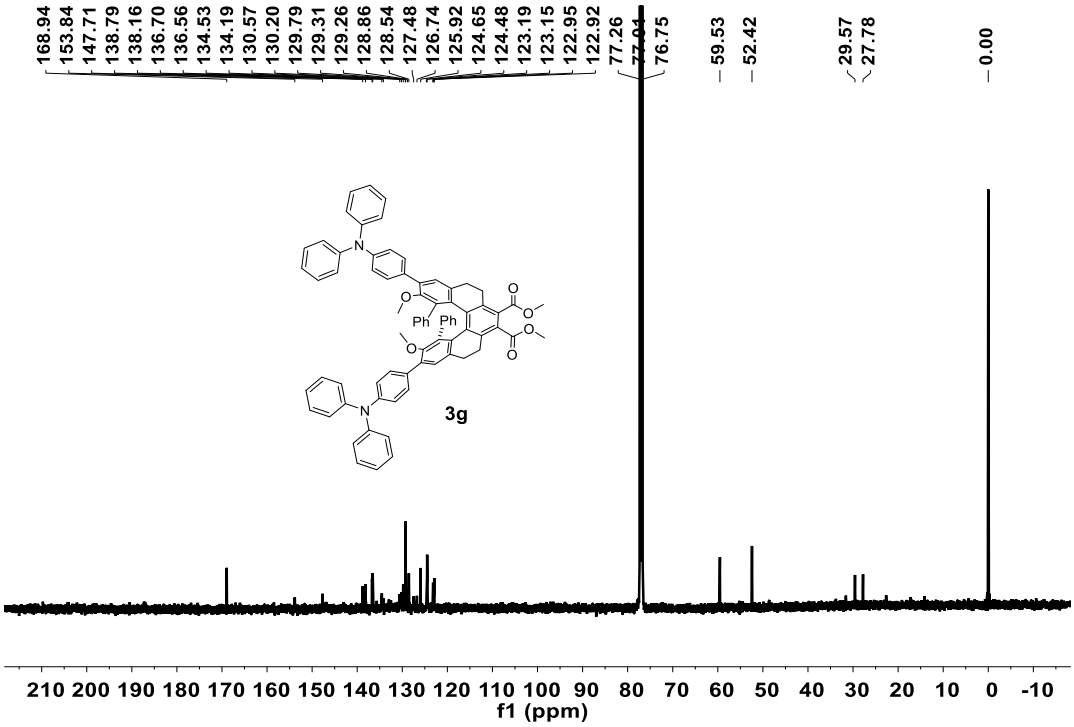


Fig. S41. ^{13}C NMR spectrum (126 MHz, CD_2Cl_2) of *P*-**3g**.

References

(1) W.-B. Lin, M. Li, L. Fang, Y. Shen and C.-F. Chen, *Chem. Asian J.,* 2017, **12**, 86.

(2) D.-Q. He, H.-Y. Lu, M. Li and C.-F. Chen, *Chem. Commun.,* 2017, **53**, 6093.

2. Crystallographic data

The single crystals of racemic **1d** and **1f** were obtained by vapor diffusion of *n*-hexane into solutions of the compounds in dichloromethane.

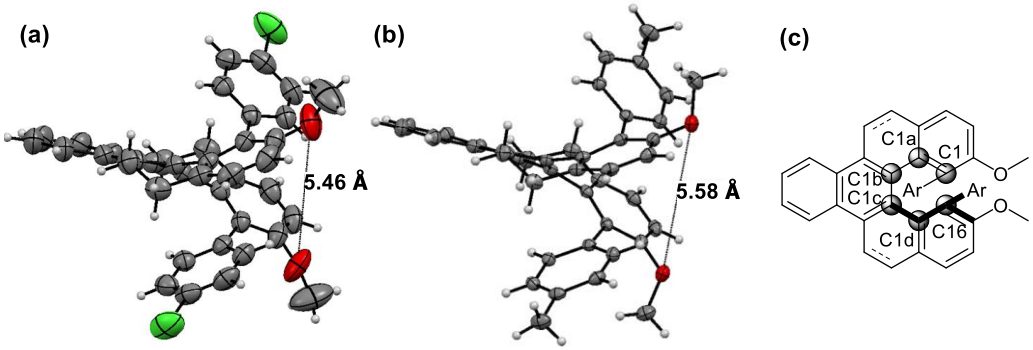


Fig. S42. ORTEP drawings and distances of the two oxygen atoms of (a) *rac*-**1d** and (b) *rac*-**1f**. (c) The presentation of distortion, which is defined by the sum of the three dihedral angles C1-C1a-C1b-C1c, C1a-C1b-C1c-C1d and C1b-C1c-C1d-C16.

Table S1. Crystal Data and Structure Refinement for 1d (CCDC 1948624).

Identification code	TX1097
Empirical formula	$C_{42}H_{36}O_2$
Formula weight	572.71
Temperature/K	170.00(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	12.36670(10)
b/Å	16.1708(2)
c/Å	15.3924(2)

α/°	90
β/°	108.8630(10)
γ/°	90
Volume/Å^3	2912.85(6)
Z	4
ρ_{calc}g/cm^3	1.306
μ/mm^{-1}	0.605
F(000)	1216.0
Crystal size/mm^3	0.3 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.17 to 150.692
Index ranges	-15 ≤ h ≤ 15, -18 ≤ k ≤ 20, -18 ≤ l ≤ 19
Reflections collected	9791
Independent reflections	2912 [R_{int} = 0.0174, R_{sigma} = 0.0160]
Data/restraints/parameters	2912/0/201
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.1032
Final R indexes [all data]	R_1 = 0.0439, wR_2 = 0.1088
Largest diff. peak/hole / e Å^{-3}	0.26/-0.23

Table S2. Crystal Data and Structure Refinement for 1f (CCDC 1948625).

Identification code	tx1102
Empirical formula	$C_{40}H_{30}Cl_2O_2$
Formula weight	613.54
Temperature/K	299.9(3)
Crystal system	monoclinic
Space group	I2/a
a/Å	12.4619(3)
b/Å	16.5737(4)

c/Å	15.2124(3)
α/°	90
β/°	103.676(2)
γ/°	90
Volume/Å^3	3052.89(12)
Z	4
ρ_{calc}g/cm^3	1.335
μ/mm^{-1}	2.189
F(000)	1280.0
Crystal size/mm^3	0.18 × 0.17 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.014 to 150.634
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 19, -18 ≤ l ≤ 18
Reflections collected	10170
Independent reflections	3000 [R_{int} = 0.0180, R_{sigma} = 0.0176]
Data/restraints/parameters	3000/0/200
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0480, wR_2 = 0.1384
Final R indexes [all data]	R_1 = 0.0528, wR_2 = 0.1445
Largest diff. peak/hole / e Å^{-3}	0.28/-0.35

3. Optical properties of new compounds

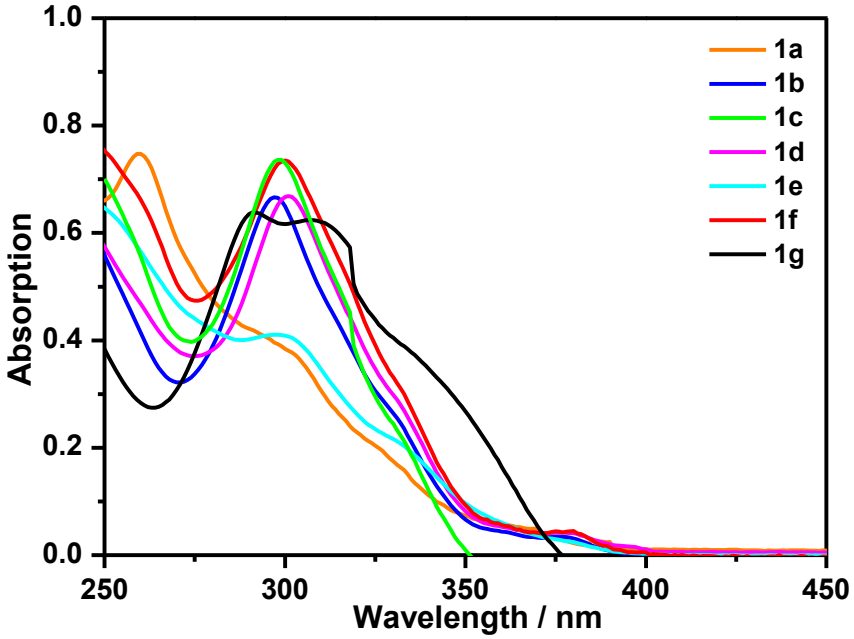


Fig. S43. UV-vis spectra of **1a~g** in CH_2Cl_2, 1.0×10^{-5} M.

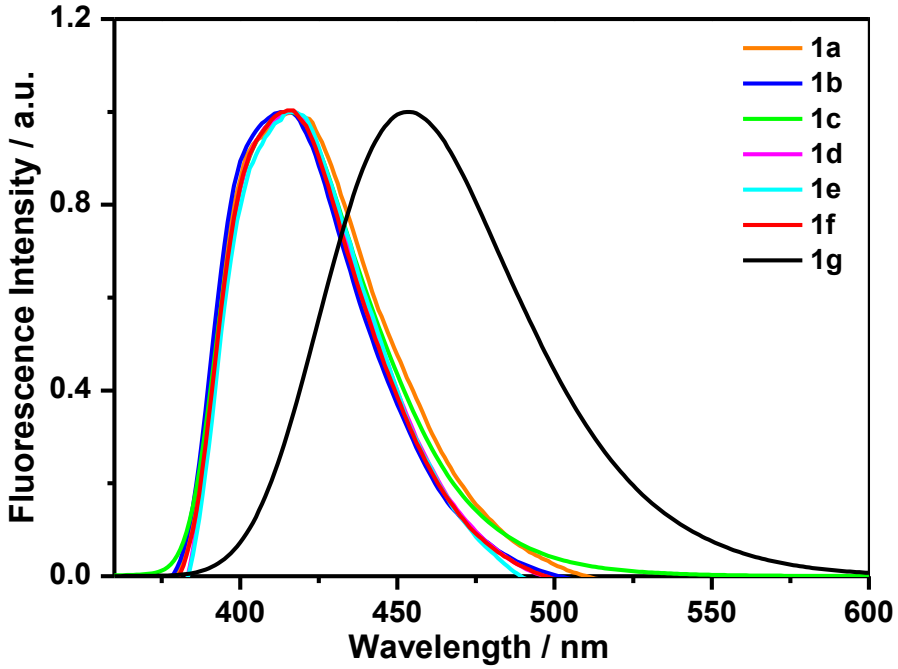


Fig. S44. Normalized fluorescence spectra of **1a~g** (excited at corresponding $\lambda_{abs,max}$) in CH_2Cl_2, 1.0×10^{-5} M.

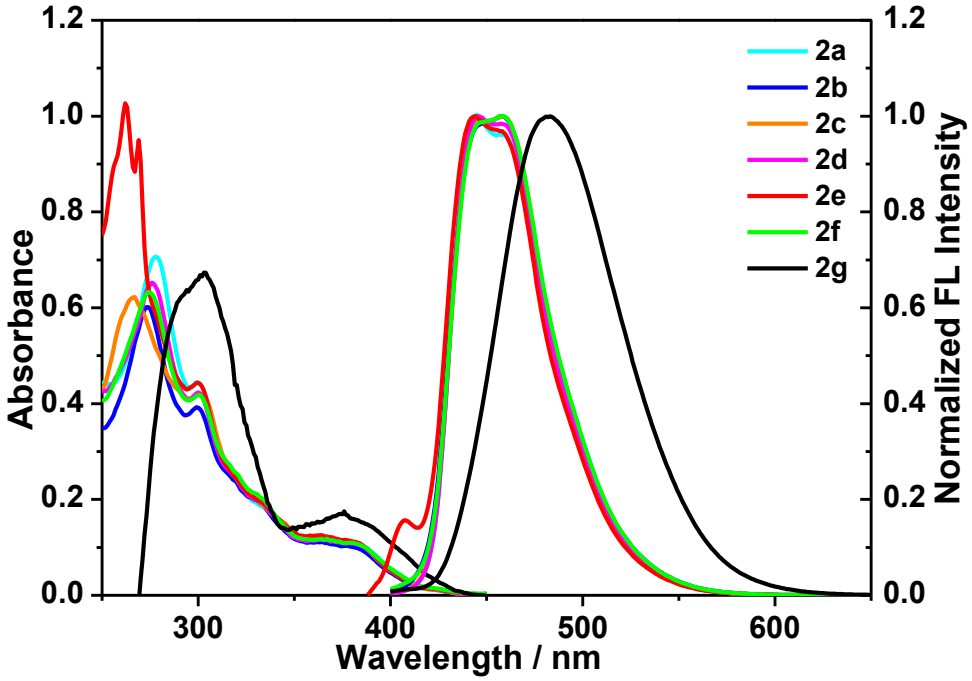


Fig. S45. UV-vis spectra and normalized fluorescence spectra of **2a~g** (excited at corresponding $\lambda_{abs,max}$) in CH_2Cl_2, 1.0×10^{-5} M.

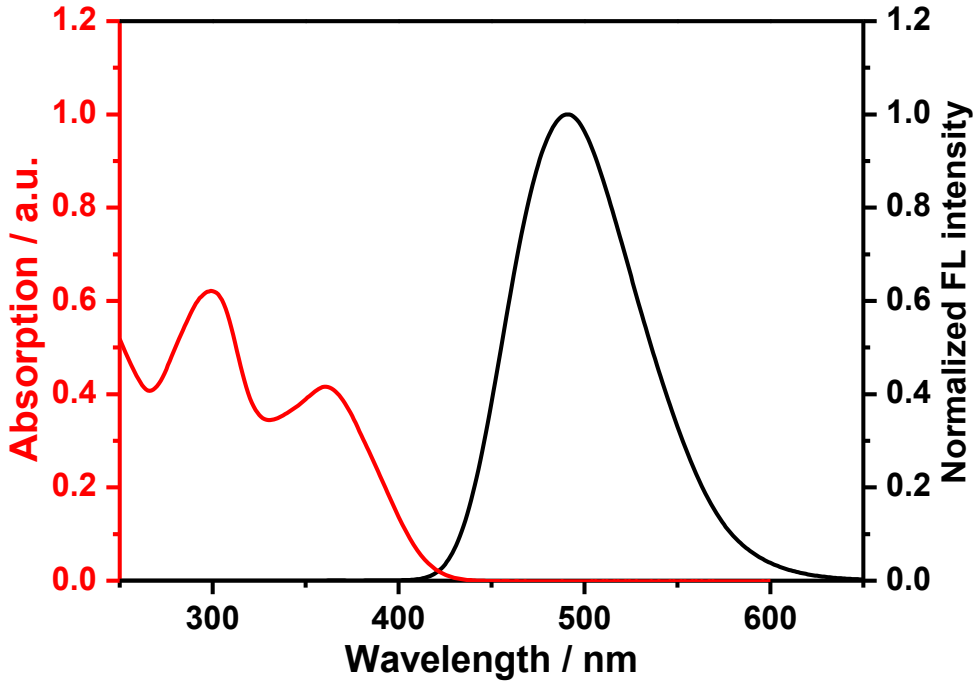


Fig. S46. UV-Vis and Normalized fluorescence spectrum (excited at corresponding $\lambda_{abs,max}$) of **3e** in THF, 5.0×10^{-5} M.

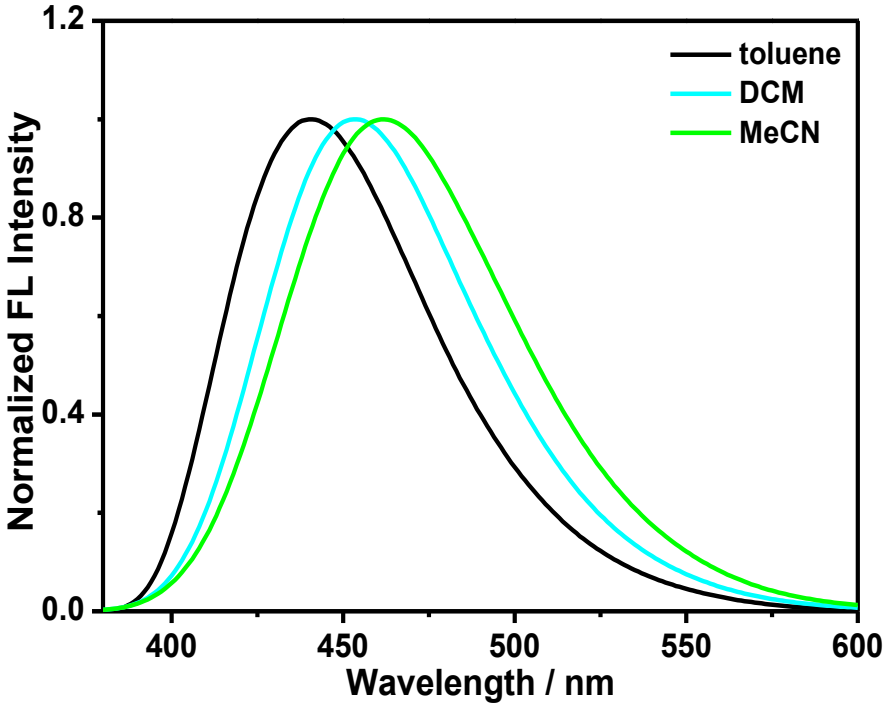


Fig. S47. Normalized fluorescence spectra of **1g** in different solvents, 10^{-4} mol·L^{-1}.

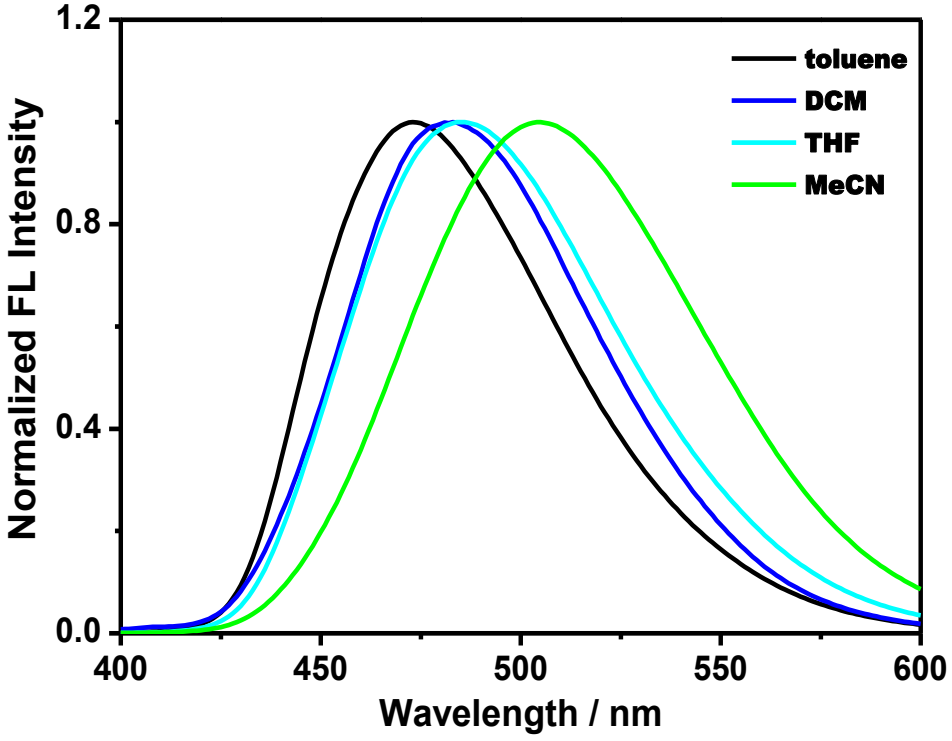


Fig. S48. Normalized fluorescence spectra of **2g** in different solvents, 10^{-4} mol·L^{-1}.

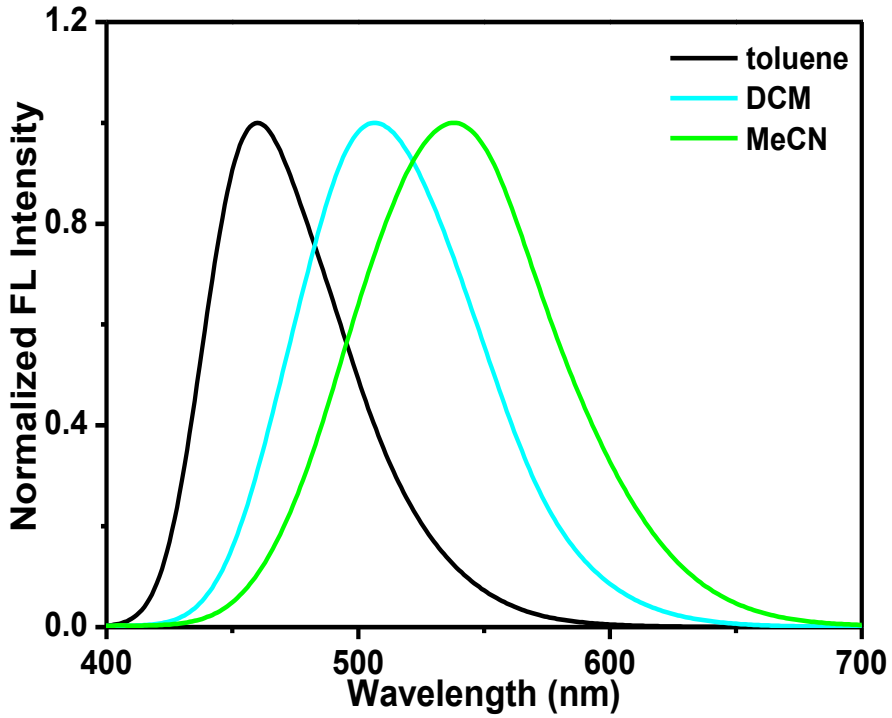


Fig. S49. Normalized fluorescence spectra of **3e** in different solvents, 10^{-4} mol·L^{-1}.

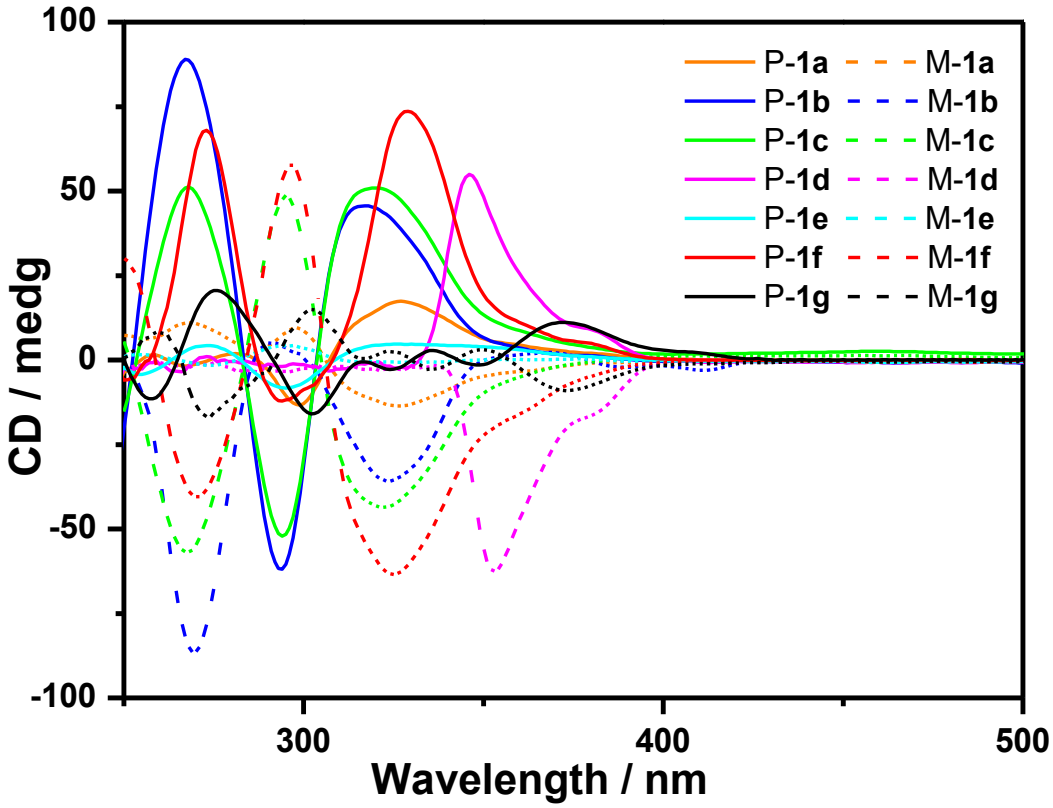


Fig. S50. CD spectra of *P*-**1** and *M*-**1** in CH_2Cl_2, 1.0×10^{-4} M.

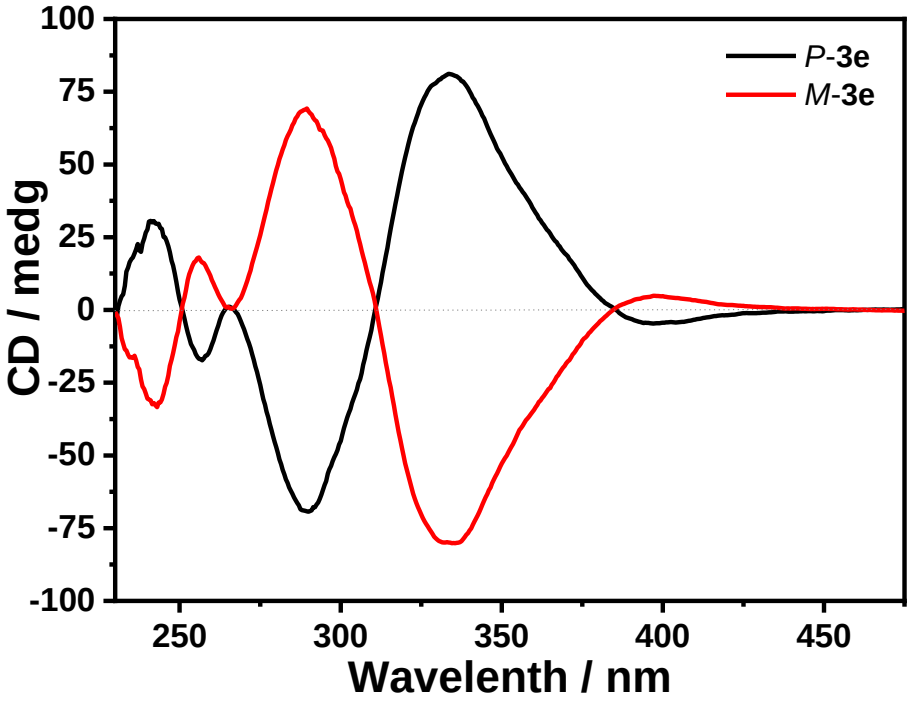


Fig. S51. CD spectra of *P*-**3e** and *M*-**3e** in THF, 5.0×10^{-5} M.

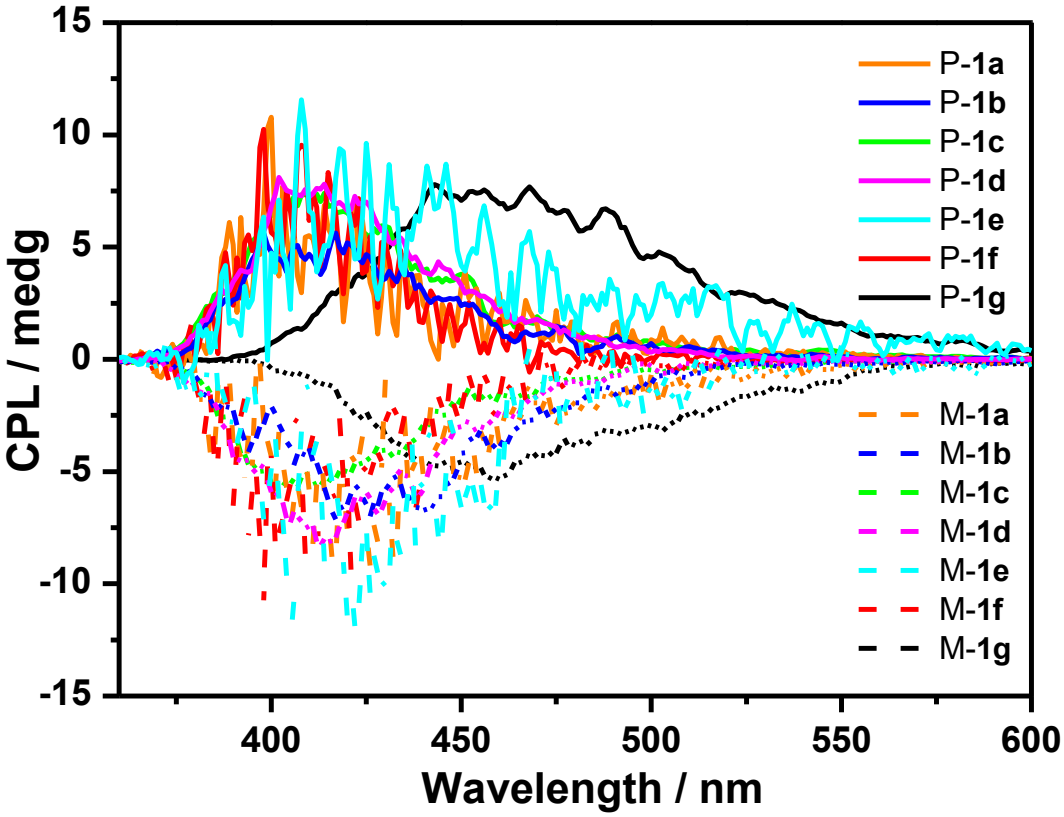


Fig. S52. CPL spectra of *P*-**1** and *M*-**1** in CH_2Cl_2, 10^{-4} mol·L^{-1}.

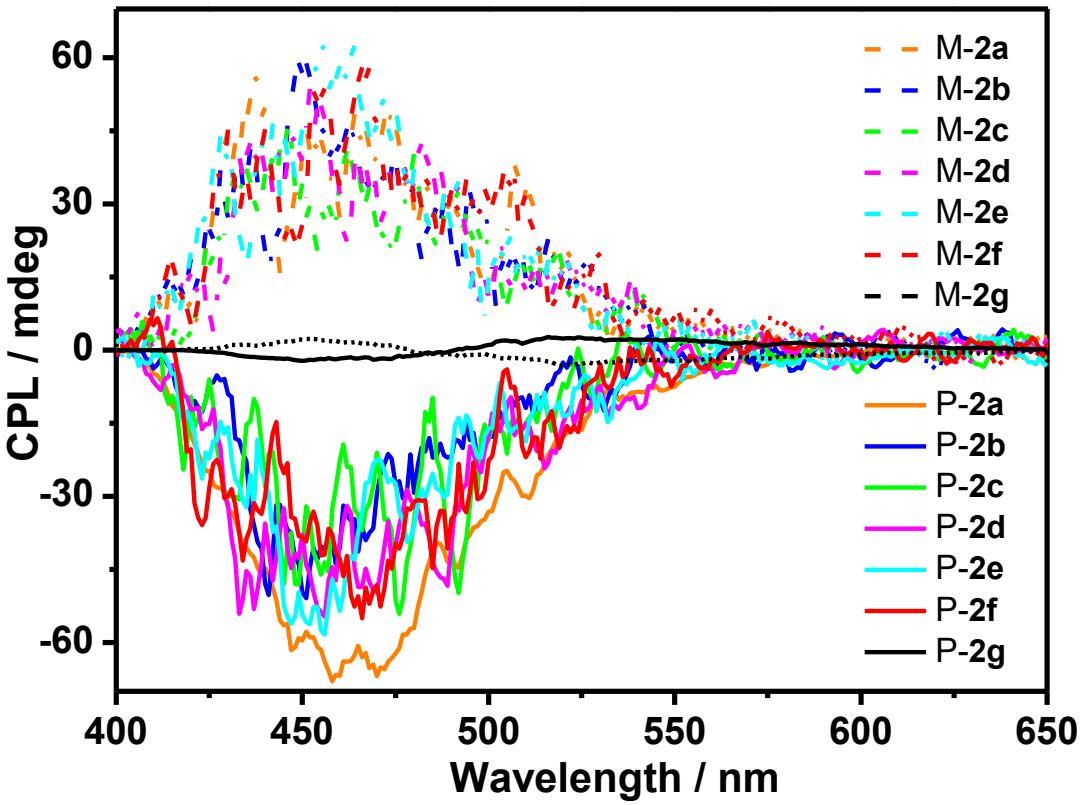


Fig. S53. CPL spectra of *P*-**2** and *M*-**2** in CH_2Cl_2, 10^{-4} mol·L^{-1}.

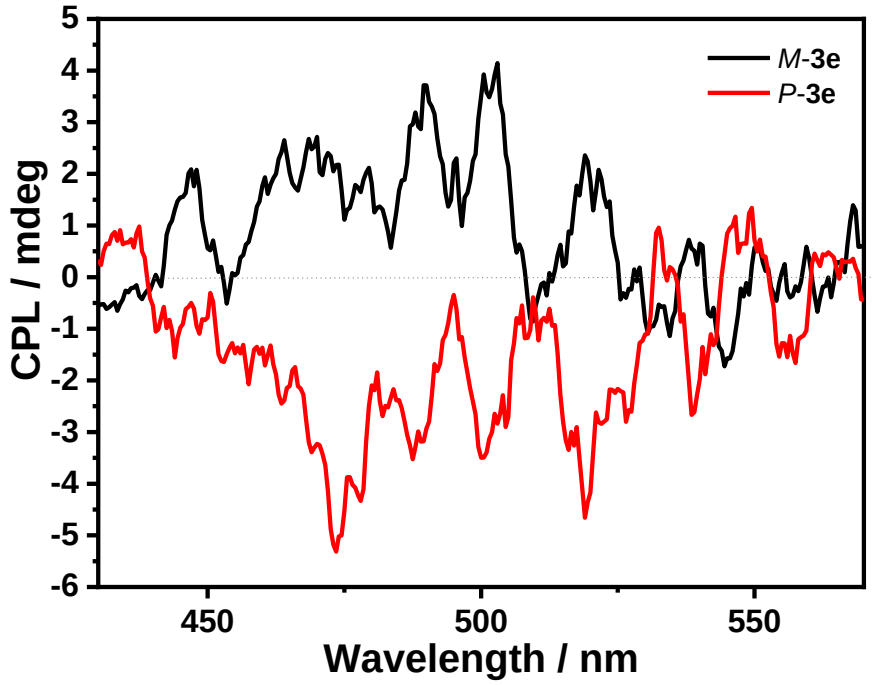


Fig. S54. CPL spectra of *P*-**3e** and *M*-**3e** in THF, 5.0×10^{-5} mol·L^{-1}.

4. DFT calculations of 1, 2 and 3

Calculations of **1**, **2** and **3** for structural optimization in ground state were performed using Gaussian09 (G09) with the 6-31+G (d, p) basis set in conjunction with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (CAM-B3LYP) density functional theory (DFT) method. Only *P* enantiomers of **1**, **2** and **3** were selected to performed relevant DFT calculations.

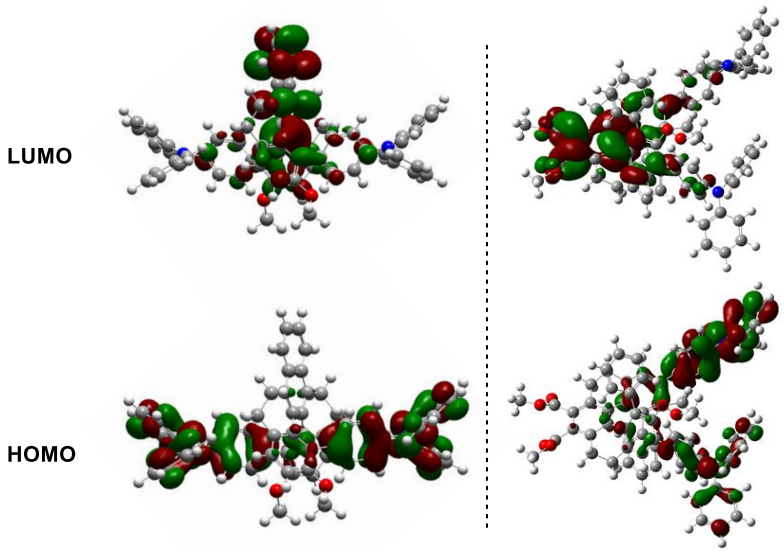


Fig. S55. Calculated spatial distributions of the HOMO and LUMO energy densities of *P*-**1g** (left) and *P*-**3e** (right) by DFT calculations.

Table S3. DFT calculation result of *P*-**1a**

C	1.80178900	-0.18031200	-2.06790800
C	2.13976600	-1.27742100	-2.83824600
C	1.28309700	-2.36777800	-2.94750000
C	0.03442500	-2.31165200	-2.34069300
C	-0.35370300	-1.19277300	-1.57027600
C	0.58402200	-0.16348800	-1.35921900
C	0.31961900	1.03409200	-0.50156300
C	0.74757900	2.25987800	-0.98600000
C	1.72901100	2.27429100	-2.13702100
C	2.64793300	1.05870300	-2.03019300

C	-0.37774700	0.97708400	0.75561300
C	-0.92772300	2.13569500	1.28027400
C	-0.60069900	3.40758600	0.72109400
C	0.29455600	3.47221300	-0.38380500
C	-0.51625700	-0.26909300	1.57306500
C	-1.72322100	-0.43291900	2.28175400
C	-2.69271600	0.71277600	2.28366600
C	-1.90399200	2.01300000	2.42876800
C	-1.08639800	4.62447500	1.27235300
C	-0.71545200	5.84141300	0.76189000
C	0.16262600	5.90516900	-0.33882700
C	0.65373700	4.75058900	-0.89109100
C	0.52187800	-1.20409800	1.75074600
C	0.25320900	-2.38087600	2.48511100
C	-0.98063900	-2.58287400	3.09113800
C	-1.94388100	-1.58244100	3.01738800
O	-0.90110400	-3.29449500	-2.49036400
C	-0.61521300	-4.38337000	-3.34363200
O	1.28420100	-3.26757300	2.60374100
C	1.11331100	-4.40644400	3.42208100
C	3.92125700	0.44951200	1.69395700
C	4.65208700	-0.46933100	0.96088700
C	4.06999400	-1.61255900	0.43798100
C	2.71657100	-1.83539200	0.65376000
C	1.94407600	-0.93141100	1.38685200
C	2.56682900	0.21143700	1.89925600
C	-2.53240000	0.01114600	-1.67379400
C	-1.79553700	-1.07741400	-1.20203200
C	-2.47665600	-2.07504200	-0.50023800
C	-3.84188200	-1.98623300	-0.27431800
C	-4.54284000	-0.89431100	-0.76327000
C	-3.90558400	0.11388100	-1.46922200
H	3.08694500	-1.28546800	-3.36983800
H	1.57325800	-3.21867000	-3.54991100
H	2.33065900	3.18345700	-2.11030400
H	3.37414600	1.04399300	-2.84753100
H	-3.40911400	0.59796700	3.10212800
H	-2.59647500	2.85544800	2.42745400
H	-1.75335800	4.59816200	2.12465200
H	-1.09742300	6.75515900	1.20570000
H	0.44939700	6.86782600	-0.74972900

H	1.31833200	4.82170200	-1.74257700
H	-1.17979300	-3.47758600	3.66629300
H	-2.88216400	-1.70378600	3.55115300
H	-0.41291100	-4.04753600	-4.36723000
H	0.23663800	-4.96882000	-2.97798100
H	-1.50838700	-5.00793900	-3.33912600
H	0.88068100	-4.12512200	4.45556100
H	0.32479000	-5.06409400	3.03766600
H	2.06560400	-4.93594800	3.39815500
H	4.40782600	1.32824900	2.10136000
O	6.03859700	-0.27224800	0.81051200
H	4.67118500	-2.31460600	-0.12795900
H	2.25375400	-2.72633100	0.24780100
H	1.98636000	0.91821000	2.48248800
H	-2.02818200	0.79265700	-2.23223200
H	-1.93032600	-2.92873100	-0.11857100
H	-4.37278800	-2.75301200	0.27829200
O	-5.92360100	-0.92608200	-0.52100900
H	-4.45179800	0.96073200	-1.86373200
C	-6.64046600	0.20189900	-0.43447800
F	-6.09511800	1.10954700	0.39774000
F	-7.85089600	-0.11246100	0.02633000
F	-6.80507000	0.81715100	-1.62460500
C	6.46278100	0.36779900	-0.28888700
F	7.78928300	0.47267000	-0.22559000
F	5.94869600	1.60872100	-0.40523900
F	6.14916100	-0.28158700	-1.42934100
H	1.20745600	2.26320700	-3.10428800
H	3.21284000	1.12221900	-1.09312100
H	-3.26555100	0.74593900	1.34948600
H	-1.38371400	2.02710400	3.39669800

Table S4. DFT calculation result of *P*-**1b**

C	0.19825800	1.63166000	-2.27463400
C	1.32296200	1.86502000	-3.04342200
C	2.36739700	0.94696700	-3.08188500
C	2.23496600	-0.25895800	-2.40461900
C	1.08484200	-0.54238700	-1.63431200
C	0.10584100	0.46028200	-1.49669600
C	-1.11777700	0.31004700	-0.64846400

C	-2.31156200	0.76995600	-1.18035400
C	-2.25592700	1.68418800	-2.38414300
C	-0.99417000	2.54247100	-2.30639700
C	-1.11719600	-0.31213100	0.64842800
C	-2.31012200	-0.77426100	1.18032700
C	-3.55436000	-0.41936400	0.57761600
C	-3.55512900	0.41277700	-0.57762100
C	0.10670600	-0.46008300	1.49665100
C	0.20131600	-1.63128900	2.27458600
C	-0.98940300	-2.54432600	2.30633000
C	-2.25275900	-1.68840400	2.38410900
C	-4.80347600	-0.81240000	1.13048400
C	-5.99150700	-0.41295700	0.57503600
C	-5.99225600	0.40193400	-0.57502800
C	-4.80495900	0.80353700	-1.13048500
C	1.08383000	0.54441500	1.63426600
C	2.23446900	0.26312600	2.40459600
C	2.36915400	-0.94254100	3.08187000
C	1.32644600	-1.86255200	3.04338300
O	3.16922100	-1.25154000	-2.48143100
C	4.28544500	-1.07234500	-3.32767000
O	3.16687700	1.25742100	2.48150800
C	4.28334000	1.08014000	3.32782500
C	-0.42144900	4.00426900	1.36062600
C	0.54220500	4.64622300	0.60586600
C	1.66273500	3.99283100	0.12536000
C	1.82435800	2.64569200	0.42438000
C	0.87980000	1.95439200	1.18719500
C	-0.24124100	2.65421300	1.64532700
C	-0.23621500	-2.65471300	-1.64530500
C	0.88349600	-1.95273900	-1.18721300
C	1.82940400	-2.64221700	-0.42442500
C	1.67038100	-3.98966100	-0.12539000
C	0.55108500	-4.64520200	-0.60584200
C	-0.41382900	-4.00510700	-1.36057300
H	1.39043000	2.77638100	-3.63068100
H	3.24207300	1.15563200	-3.68394900
H	-3.13258300	2.33274600	-2.40724200
H	-0.92873800	3.21820900	-3.16402700
H	-0.92270100	-3.21995300	3.16395000
H	-3.12819000	-2.33861100	2.40722900

H	-4.82501100	-1.42922200	2.01991400
H	-6.93080500	-0.72340900	1.02138100
H	-6.93212100	0.71067700	-1.02136400
H	-4.82761500	1.42032400	-2.01991400
H	3.24421400	-1.14955500	3.68395800
H	1.39561400	-2.77378600	3.63064100
H	3.97799800	-0.91278200	-4.36770900
H	4.90908100	-0.23203500	-3.00014600
H	4.86201300	-1.99480900	-3.25989000
H	4.85827900	2.00362800	3.26016100
H	3.97608200	0.91995000	4.36782400
H	4.90848000	0.24095200	3.00028800
H	-1.28498100	4.55263300	1.71939800
H	2.38934700	4.53410000	-0.46982800
H	2.69800200	2.12195200	0.05589500
H	-0.98130600	2.13726300	2.24717500
H	-0.97728600	-2.13919300	-2.24714100
H	2.70205800	-2.11679400	-0.05598600
H	2.39805600	-4.52952900	0.46977200
F	0.39355000	-5.96282800	-0.32260900
H	-1.27631900	-4.55513100	-1.71930800
F	0.38212800	5.96354600	0.32265100
H	-2.25769800	1.10953100	-3.32092700
H	-1.03860000	3.16135100	-1.40229100
H	-1.03267300	-3.16327600	1.40221300
H	-2.25558000	-1.11376100	3.32089800

Table S5. DFT calculation result of *P*-**1c**

C	0.23988200	1.77816500	-2.17015200
C	1.36494400	2.03996300	-2.91602700
C	2.40116000	1.11701800	-3.00824100
C	2.26299200	-0.12204400	-2.39778200
C	1.10842100	-0.44561400	-1.66195100
C	0.12164600	0.55105800	-1.47232800
C	-1.04846900	0.37900400	-0.61275800
C	-2.27269800	0.97881300	-1.02277000
C	-2.21803900	2.04916200	-2.07441700
C	-0.87489600	2.76949600	-2.04743000
C	-1.04844100	-0.37908000	0.61273900
C	-2.27263100	-0.97896500	1.02276200

C	-3.50395100	-0.53572400	0.49505800
C	-3.50398900	0.53548600	-0.49506400
C	0.12169100	-0.55106100	1.47229700
C	0.24000800	-1.77815300	2.17013900
C	-0.87470900	-2.76955400	2.04743000
C	-2.21789700	-2.04930100	2.07441800
C	-4.74895900	-1.02735700	0.94159000
C	-5.94507200	-0.51940300	0.47404000
C	-5.94510900	0.51899100	-0.47404200
C	-4.74903200	1.02703100	-0.94159300
C	1.10837500	0.44569400	1.66194300
C	2.26294000	0.12223300	2.39783500
C	2.40120200	-1.11681800	3.00829100
C	1.36507600	-2.03985700	2.91603800
O	3.19536200	-1.10666600	-2.52127300
C	4.30825800	-0.88977800	-3.35576900
O	3.19522400	1.10692500	2.52139200
C	4.30805800	0.89009300	3.35598200
C	-0.45434700	3.87603800	1.65988400
C	0.48212100	4.63056400	0.96676000
C	1.60613700	4.00695100	0.44131700
C	1.80220800	2.64633800	0.62049400
C	0.87679500	1.87773500	1.32555100
C	-0.25823000	2.51384600	1.83276300
C	-0.25791800	-2.51393600	-1.83288300
C	0.87698000	-1.87767500	-1.32557000
C	1.80245500	-2.64617700	-0.62048200
C	1.60655600	-4.00682200	-0.44135100
C	0.48266100	-4.63057700	-0.96688200
C	-0.45385800	-3.87615900	-1.66005500
H	1.45393300	2.99169900	-3.43044100
H	3.28023200	1.35768600	-3.58980400
H	-2.37644800	1.60200900	-3.06565100
H	-0.78492900	3.31874100	-1.10560500
H	-0.81895100	-3.50458100	2.85379400
H	-3.02386000	-2.76920000	1.92709800
H	-4.77777600	-1.81167300	1.68653200
H	-6.88236100	-0.91934800	0.84298200
H	-6.88242600	0.91887000	-0.84298300
H	-4.77790800	1.81134500	-1.68653400
H	3.28027400	-1.35740000	3.58989300

H	1.45412600	-2.99157900	3.43046700
H	4.87841000	-1.81602600	-3.33863800
H	4.00420200	-0.67308400	-4.38451800
H	4.93872600	-0.07414100	-2.98731900
H	4.87814700	1.81638100	3.33892900
H	4.00392200	0.67334800	4.38469700
H	4.93861600	0.07450900	2.98756700
H	-1.33736800	4.34911600	2.07611200
H	0.33655900	5.69750900	0.83546200
H	2.33968200	4.58504300	-0.11056200
H	2.68379000	2.17042700	0.21195700
H	-0.98390400	1.93290400	2.39064200
H	-0.98362500	-1.93309000	-2.39081900
H	2.68395800	-2.17016600	-0.21189100
H	2.34014700	-4.58482600	0.11055900
H	0.33723900	-5.69754500	-0.83562400
H	-1.33678100	-4.34934700	-2.07636800
H	-3.02404500	2.76901000	-1.92707800
H	-0.81918300	3.50453600	-2.85378500
H	-0.78471400	-3.31880200	1.10561200
H	-2.37632200	-1.60214300	3.06564800

Table S6. DFT calculation result of *P*-**1d**

C	1.58907800	-0.31137700	-2.28794000
C	1.74546800	-1.44823800	-3.05794000
C	0.76310300	-2.43296300	-3.08753100
C	-0.42698300	-2.22472900	-2.40147000
C	-0.63328300	-1.05827400	-1.63103500
C	0.43189000	-0.14658400	-1.50136000
C	0.36575100	1.08280400	-0.65176500
C	0.89322200	2.24697700	-1.18488900
C	1.79664900	2.13647200	-2.39295500
C	2.57306000	0.82151600	-2.32304100
C	-0.24380600	1.11695600	0.64968400
C	-0.63794800	2.33291900	1.18277200
C	-0.21574700	3.55504600	0.57840300
C	0.61248500	3.50849600	-0.57913100
C	-0.44670900	-0.09665200	1.50008300
C	-1.61546500	-0.13118300	2.28606600
C	-2.46821100	1.10344500	2.31674900

C	-1.55058500	2.32388400	2.38904200
C	-0.53503600	4.82439000	1.13233500
C	-0.06836300	5.98802600	0.57710000
C	0.74358300	5.94243000	-0.57417200
C	1.07412900	4.73402000	-1.13141900
C	0.51125300	-1.12007600	1.63246800
C	0.17808600	-2.25401600	2.40685500
C	-1.02753100	-2.32778700	3.09357700
C	-1.89604800	-1.24139800	3.05961300
O	-1.47677000	-3.09539100	-2.47118600
C	-1.36858600	-4.22634900	-3.30808700
O	1.12589800	-3.23453100	2.47980600
C	0.89493000	-4.34213600	3.32287200
C	4.03891700	0.20795800	1.33541600
C	4.68646700	-0.76335300	0.57398900
C	3.92665700	-1.84224500	0.11336700
C	2.57596000	-1.95344100	0.41102900
C	1.92700200	-0.98226200	1.17798500
C	2.68283400	0.10127000	1.63094100
C	-2.65642600	0.39629700	-1.62881500
C	-2.02519900	-0.76450200	-1.17694900
C	-2.77756900	-1.65816700	-0.40983400
C	-4.10805600	-1.39952700	-0.11365800
C	-4.74483500	-0.24439800	-0.57651000
C	-3.99294300	0.65144200	-1.33420800
H	2.64640800	-1.57348900	-3.65193200
H	0.91203200	-3.31990100	-3.68942000
H	2.49972400	2.97036700	-2.41555800
H	3.23711500	0.71558300	-3.18613700
H	-3.14327400	1.07272100	3.17725300
H	-2.15641300	3.23099000	2.41075800
H	-1.14819800	4.88028800	2.02297200
H	-0.32318900	6.94342800	1.02466400
H	1.10593400	6.86317600	-1.02023200
H	1.68954300	4.72102700	-2.02216300
H	-1.27321900	-3.19058400	3.69892200
H	-2.80556000	-1.26509700	3.65322500
H	-1.19664000	-3.93848500	-4.35201900
H	-0.56493000	-4.89652300	-2.97982900
H	-2.32325200	-4.74686400	-3.23098000
H	0.75604700	-4.03135100	4.36515700

H	0.02240600	-4.92190600	2.99830000
H	1.78672400	-4.96461200	3.24869100
H	4.60095400	1.05836200	1.71205700
H	6.62662100	0.15575500	0.80458200
H	4.40288700	-2.61287900	-0.48773700
H	2.01458900	-2.80444100	0.04340200
H	2.20687900	0.86523400	2.23770700
H	-2.09835800	1.10478900	-2.23286300
H	-2.31251900	-2.56442200	-0.03984600
H	-4.66597200	-2.11210500	0.48881200
C	-6.19751000	0.01255200	-0.26762000
H	-4.45686800	1.56020100	-1.70814800
H	6.30736100	-0.45625200	-0.82143700
H	6.68388000	-1.58207400	0.48173800
H	-6.83852300	-0.75623500	-0.71168800
H	-6.52082900	0.98108300	-0.65681200
H	-6.38338900	0.00537800	0.81133900
C	6.15325600	-0.65474400	0.24493300
H	1.21931600	2.17849600	-3.32722400
H	3.19768900	0.82204900	-1.42164300
H	-3.08550800	1.17193500	1.41290600
H	-0.97412900	2.30075500	3.32452600

Table S7. DFT calculation result of *P*-**1e**

C	1.84755200	0.44007500	-2.14936000
C	2.43925300	-0.60431700	-2.87969000
C	1.85178500	-1.83998200	-2.94693600
C	0.59703800	-2.03640300	-2.34193100
C	-0.02819300	-1.03405700	-1.59453300
C	0.66524800	0.20297900	-1.39401600
C	0.19164300	1.29151200	-0.54406700
C	0.58816100	2.59818500	-0.85724700
C	1.72477400	2.80506000	-1.69575900
C	2.38621900	1.75402800	-2.23723500
C	-0.69343700	1.10334900	0.60092300
C	-1.57832400	2.14091200	0.92271500
C	-1.33430400	3.48609600	0.41938400
C	-0.17414900	3.73049900	-0.34803300
C	-0.68887600	-0.08833300	1.44389700
C	-1.86431000	-0.34862300	2.20169000

C	-2.88167900	0.64078100	2.30209000
C	-2.69778400	1.87199800	1.76673900
C	-2.15793900	4.57784300	0.76669800
C	-1.83738600	5.86790300	0.40479200
C	-0.66570100	6.11451500	-0.32090900
C	0.14376400	5.06226100	-0.68891500
C	0.44272000	-0.94631100	1.63340300
C	0.27085100	-2.12223000	2.37021400
C	-0.95624200	-2.44742100	2.97658700
C	-1.98807300	-1.54870600	2.92228600
O	-0.09377700	-3.20120900	-2.51092600
C	0.39002900	-4.17167900	-3.41601900
O	1.36672700	-2.92073700	2.52669900
C	1.31301600	-4.00537100	3.43041100
C	3.63546700	1.08068400	1.49310100
C	4.51420000	0.21146200	0.84502300
C	4.05924900	-1.03410000	0.42085900
C	2.73328700	-1.39641700	0.64665600
C	1.83793000	-0.54431900	1.28752200
C	2.32243300	0.70177800	1.71120900
C	-2.41104600	-0.29832400	-1.66584300
C	-1.46592700	-1.23201200	-1.24554000
C	-1.93630900	-2.37899400	-0.59323700
C	-3.28542900	-2.57380800	-0.36129800
C	-4.21522300	-1.62071900	-0.78094100
C	-3.77511200	-0.47594400	-1.43904400
H	3.36446100	-0.41089100	-3.41436200
H	2.32106800	-2.63042500	-3.51778700
H	2.09839900	3.80571000	-1.86467200
H	3.29400900	1.90719700	-2.81311000
H	-3.77041200	0.41496300	2.88384900
H	-3.43625900	2.64093900	1.94875000
H	-3.05751700	4.41624600	1.34588500
H	-2.48760100	6.68827400	0.69110300
H	-0.39771600	7.12802000	-0.60142700
H	1.03320000	5.27663200	-1.26651600
H	-1.07051300	-3.36609900	3.53656900
H	-2.91325300	-1.74754200	3.45469200
H	-0.36675400	-4.95582900	-3.44087300
H	0.51332500	-3.75639600	-4.42277900
H	1.34054600	-4.60268100	-3.08017700

H	1.03963000	-3.67517900	4.43903500
H	0.61079900	-4.77821800	3.09658200
H	2.31936300	-4.42397000	3.44970000
H	4.00374800	2.04583500	1.82326600
O	5.78993500	0.66686300	0.67550100
H	4.71526000	-1.72879900	-0.08859200
H	2.39483900	-2.36746600	0.30780300
H	1.65613600	1.38431800	2.22882000
H	-2.08236800	0.59347300	-2.18985100
H	-1.23022900	-3.12766800	-0.25656200
H	-3.64385700	-3.45948700	0.15206000
O	-5.52264600	-1.89628800	-0.50153900
H	-4.46980900	0.28055300	-1.78151700
C	-6.50425000	-0.96942800	-0.91726500
H	-6.35685300	0.00909700	-0.44527800
H	-7.46228900	-1.38170400	-0.60068500
H	-6.50469300	-0.84882600	-2.00702100
C	6.72834900	-0.18680100	0.05586900
H	7.66998600	0.36187800	0.03741000
H	6.43244200	-0.43135200	-0.97137800
H	6.86136800	-1.11533900	0.62368000

Table S8. DFT calculation result of *P*-**1f**

C	1.61591600	-0.18912100	-2.28661300
C	1.84151700	-1.31407900	-3.05769700
C	0.92187100	-2.35716200	-3.08989200
C	-0.27868200	-2.22375800	-2.40318200
C	-0.55394500	-1.07340500	-1.63054100
C	0.45054000	-0.09505300	-1.50030300
C	0.30771600	1.12810500	-0.65013300
C	0.76621900	2.32134700	-1.18445800
C	1.67331000	2.26511200	-2.39362700
C	2.52919600	1.00123700	-2.32378300
C	-0.30771300	1.12811200	0.65013900
C	-0.76622200	2.32135900	1.18444300
C	-0.41331600	3.56516800	0.57960500
C	0.41332500	3.56516400	-0.57962600
C	-0.45055000	-0.09503400	1.50031600
C	-1.61590500	-0.18909600	2.28661100
C	-2.52919200	1.00126100	2.32381000

C	-1.67332300	2.26514600	2.39360500
C	-0.80270100	4.81459400	1.13430800
C	-0.40478600	6.00219300	0.57689300
C	0.40482600	6.00219000	-0.57690000
C	0.80272600	4.81458800	-1.13432000
C	0.55394800	-1.07340500	1.63055700
C	0.27868300	-2.22373900	2.40317400
C	-0.92191100	-2.35716400	3.08986000
C	-1.84153600	-1.31408900	3.05767200
O	-1.27319300	-3.15609600	-2.47270400
C	-1.10415000	-4.27076000	-3.32351800
O	1.27320200	-3.15607500	2.47272300
C	1.10418800	-4.27071800	3.32356700
C	4.00796500	0.43528000	1.31961500
C	4.66244300	-0.52320200	0.55871100
C	3.99072600	-1.64700800	0.09521600
C	2.64782100	-1.81353000	0.40747500
C	1.96007400	-0.86970900	1.17285900
C	2.66215600	0.25413100	1.61880000
C	-2.66215700	0.25411400	-1.61880900
C	-1.96008000	-0.86971600	-1.17284200
C	-2.64783100	-1.81351900	-0.40744000
C	-3.99073600	-1.64699100	-0.09519400
C	-4.66245200	-0.52319400	-0.55871800
C	-4.00797100	0.43527000	-1.31963600
H	2.74858000	-1.38274100	-3.65140100
H	1.12476100	-3.23188700	-3.69382700
H	2.32389900	3.14015900	-2.41904700
H	3.19810100	0.93533400	-3.18663100
H	-3.19804400	0.93536200	3.18670000
H	-2.32392600	3.14018600	2.41898100
H	-1.41550100	4.83670500	2.02647700
H	-0.71244100	6.94177700	1.02452800
H	0.71249500	6.94177200	-1.02452800
H	1.41553200	4.83669900	-2.02648400
H	-1.12480800	-3.23191300	3.69375200
H	-2.74862200	-1.38274100	3.65134300
H	-0.95321100	-3.96077000	-4.36402000
H	-0.26249100	-4.89708900	-3.00492400
H	-2.02737500	-4.84518700	-3.24889800
H	0.95304900	-3.96068100	4.36402800

H	0.26266200	-4.89718500	3.00489000
H	2.02749600	-4.84503200	3.24910400
H	4.54255100	1.30754900	1.67789400
H	4.51335300	-2.38372000	-0.50411300
H	2.12539800	-2.69101500	0.04614300
H	2.15096800	0.99643300	2.22292900
H	-2.15096800	0.99640400	-2.22295200
H	-2.12540400	-2.69098800	-0.04607300
H	-4.51336900	-2.38369200	0.50414400
Cl	-6.35760400	-0.31132400	-0.17495200
H	-4.54255000	1.30753300	-1.67794100
Cl	6.35759300	-0.31133600	0.17493600
H	1.09285800	2.27029500	-3.32681900
H	3.15569400	1.04256300	-1.42488200
H	-3.15574600	1.04256700	1.42494800
H	-1.09287900	2.27038000	3.32680200

Table S9. DFT calculation result of *P*-**1g**

C	-1.53539100	-0.01619200	2.33471600
C	-1.75473400	-1.14592800	3.09945600
C	-0.84819400	-2.20029000	3.09109700
C	0.33237200	-2.07488400	2.36968500
C	0.60219000	-0.92144400	1.59703400
C	-0.39530800	0.06965500	1.51083400
C	-0.27482400	1.29784800	0.66385100
C	-0.69939000	2.49295700	1.22261100
C	-1.54722300	2.43641800	2.47332700
C	-2.42661100	1.18873000	2.41846600
C	0.27482700	1.29764300	-0.66421300
C	0.69940000	2.49257800	-1.22333900
C	0.37856600	3.73685200	-0.60326500
C	-0.37855100	3.73703900	0.60215400
C	0.39531200	0.06918900	-1.51081700
C	1.53540300	-0.01691700	-2.33466000
C	2.42662600	1.18797800	-2.41877600
C	1.54724000	2.43565000	-2.47403300
C	0.73346700	4.98655800	-1.18074000
C	0.36937300	6.17426500	-0.60123900
C	-0.36934400	6.17445100	0.59938200
C	-0.73344400	4.98692300	1.17924600

C	-0.60218900	-0.92193300	-1.59671800
C	-0.33236200	-2.07561700	-2.36900300
C	0.84821200	-2.20125200	-3.09036200
C	1.75475400	-1.14689300	-3.09904300
O	1.31402400	-3.02373800	2.40555700
C	1.14473300	-4.14840500	3.24136100
O	-1.31401500	-3.02448100	-2.40459600
C	-1.14470900	-4.14941000	-3.24004500
C	-4.06478100	0.54027400	-1.15470500
C	-4.73308000	-0.45546800	-0.43711300
C	-4.00806100	-1.57701500	-0.02368700
C	-2.66411500	-1.70634500	-0.34178000
C	-1.99417700	-0.73602300	-1.09095700
C	-2.72345500	0.39120600	-1.48235600
C	2.66410000	-1.70628800	0.34234300
C	1.99417200	-0.73570600	1.09119200
C	2.72345600	0.39165400	1.48219700
C	4.06477900	0.54060700	1.15448000
C	4.73306900	-0.45538500	0.43722700
C	4.00804400	-1.57707300	0.02419800
N	-6.11747500	-0.33253200	-0.15460500
N	6.11746600	-0.33256100	0.15467700
C	6.65028000	-0.80747100	-1.06853700
C	6.99493800	0.18261700	1.14363300
C	-6.65028100	-0.80704800	1.06877100
C	-6.99496300	0.18223800	-1.14375400
C	8.00028100	1.08727400	0.78957500
C	8.86849600	1.58534800	1.75377300
C	8.73836900	1.20396300	3.08659200
C	7.73235100	0.30978700	3.44287300
C	6.87115200	-0.20539000	2.48096100
C	7.85113700	-1.52444100	-1.09102400
C	8.37828500	-1.97674200	-2.29510200
C	7.71247700	-1.73879000	-3.49412500
C	6.51221500	-1.03304600	-3.47367600
C	5.98759900	-0.56340100	-2.27578000
C	-7.85107100	-1.52412000	1.09149400
C	-8.37819900	-1.97603000	2.29572900
C	-7.71243400	-1.73757800	3.49467600
C	-6.51223600	-1.03173100	3.47399200
C	-5.98764200	-0.56247600	2.27593500

C	-8.00038400	1.08693800	-0.79002000
C	-8.86862100	1.58461900	-1.75440100
C	-8.73844300	1.20279500	-3.08708900
C	-7.73235000	0.30857600	-3.44305000
C	-6.87112600	-0.20620900	-2.48095000
H	-2.64425000	-1.21115400	3.71957300
H	-1.04501700	-3.07955100	3.69032000
H	-2.17927100	3.32227300	2.54441100
H	-3.06324800	1.12417900	3.30617900
H	3.06327100	1.12315000	-3.30646300
H	2.17929100	3.32148100	-2.54538700
H	1.29171800	5.00891800	-2.10801800
H	0.64929400	7.11373400	-1.06705200
H	-0.64925800	7.11406500	1.06490700
H	-1.29169400	5.00957100	2.10651700
H	1.04504100	-3.08070100	-3.68930700
H	2.64427600	-1.21231500	-3.71913000
H	1.02622700	-3.85434300	4.29091600
H	0.28308500	-4.75351600	2.93493700
H	2.05427200	-4.73947300	3.13343500
H	-2.05424900	-4.74044500	-3.13194800
H	-1.02618500	-3.85567600	-4.28969000
H	-0.28306500	-4.75442400	-2.93341700
H	-4.60401900	1.42396000	-1.47795000
H	-4.50337300	-2.35767900	0.54293000
H	-2.12982900	-2.59057000	-0.01599700
H	-2.23448500	1.16697600	-2.06289700
H	2.12980900	-2.59062700	0.01687400
H	2.23449300	1.16762600	2.06247500
H	4.60402200	1.42440300	1.47741900
H	4.50335000	-2.35793600	-0.54215100
H	8.09724800	1.39497800	-0.24604100
H	9.64383800	2.28663000	1.46127500
H	9.41243100	1.59987900	3.83896200
H	7.62125900	-0.00049000	4.47724500
H	6.09353300	-0.90729500	2.76164300
H	8.37095000	-1.72282900	-0.16021100
H	9.31205600	-2.53049600	-2.29157800
H	8.12344100	-2.09750800	-4.43192700
H	5.98434100	-0.83191900	-4.40103100
H	5.05836000	-0.00620300	-2.26749500

H	-8.37084700	-1.72289400	0.16074400
H	-9.31191800	-2.52987100	2.29239100
H	-8.12338200	-2.09599100	4.43260100
H	-5.98439800	-0.83021800	4.40128400
H	-5.05845300	-0.00519600	2.26745800
H	-8.09739300	1.39498600	0.24549000
H	-9.64402100	2.28594000	-1.46215100
H	-9.41252200	1.59840500	-3.83960400
H	-7.62121700	-0.00204200	-4.47731500
H	-6.09345000	-0.90815000	-2.76138600
H	3.08036700	1.25415500	-1.54009000
H	0.92387600	2.41089200	-3.37865500
H	-0.92385300	2.41194000	3.37795300
H	-3.08036000	1.25463300	1.53976500

Table S10. DFT calculation result of *P*-**2a**

C	-1.76696000	0.46831200	2.42626900
C	-2.23205200	-0.58652600	3.23095600
C	-1.52422000	-1.75265200	3.34673400
C	-0.27490200	-1.86304300	2.70841400
C	0.22320700	-0.85013000	1.88414200
C	-0.58781800	0.30701900	1.64654100
C	-0.24506900	1.38845500	0.72870600
C	-0.76281100	2.66509000	0.98720300
C	-1.89609900	2.80321900	1.84300200
C	-2.43561000	1.72323000	2.45860500
C	0.63326800	1.22976400	-0.42654900
C	1.40771600	2.33116100	-0.81605900
C	1.04157800	3.67000000	-0.37200600
C	-0.12510800	3.83913800	0.40525100
C	0.72856000	0.00619000	-1.21565700
C	1.90651000	-0.17288600	-1.99293800
C	2.82532800	0.90049100	-2.15516200
C	2.53430200	2.13110900	-1.66830300
C	1.75030400	4.81670900	-0.78798100
C	1.31038900	6.08600500	-0.48281400
C	0.13057300	6.25427700	0.25182800
C	-0.56711000	5.14894900	0.68693600
C	-0.31191100	-0.97163200	-1.33533700
C	-0.04867300	-2.15129900	-2.03709000

C	1.18926800	-2.37974300	-2.66635000
C	2.12974600	-1.38487300	-2.67009000
O	0.52923800	-2.94487900	2.91369200
C	0.17523800	-3.90091800	3.89447500
O	-1.06610000	-3.05373200	-2.13288000
C	-0.93877500	-4.15834800	-3.00768400
C	-3.70174900	0.70175700	-1.13507400
C	-4.41846300	-0.23666900	-0.41318100
C	-3.83010800	-1.40085900	0.05082100
C	-2.48910300	-1.63071500	-0.22455900
C	-1.73111900	-0.70914000	-0.95180000
C	-2.36159500	0.45348900	-1.40677500
C	2.53003900	0.10432000	1.81969700
C	1.65995800	-0.93870500	1.48605900
C	2.19476800	-2.07524200	0.87349200
C	3.54982400	-2.16695700	0.58692800
C	4.37631000	-1.10591800	0.91463200
C	3.88877400	0.03034100	1.53648800
H	-3.15859400	-0.45518100	3.78165000
H	-1.89710200	-2.55106200	3.97434700
H	-2.36381600	3.76978200	1.97070300
H	-3.34129600	1.81602900	3.05014300
H	3.72480600	0.73281000	-2.73903900
H	3.19662700	2.95543300	-1.89402100
H	2.65337100	4.71380600	-1.37479900
H	1.87357700	6.94995600	-0.82029100
H	-0.23080700	7.24995200	0.48748300
H	-1.46423400	5.30590500	1.27099500
H	1.37782100	-3.30385800	-3.19644800
H	3.05950700	-1.51477500	-3.21536000
H	0.04787400	-3.43654500	4.87854100
H	-0.73896800	-4.44068600	3.62255500
H	1.00628600	-4.60489600	3.93325700
H	-0.72566000	-3.83474000	-4.03237300
H	-0.15956800	-4.85247900	-2.67291800
H	-1.90279500	-4.66606600	-2.98323500
H	-4.18703300	1.60733800	-1.47992600
O	-5.75725200	0.03562600	-0.07122600
H	-4.41528200	-2.10979600	0.62501000
H	-2.02265800	-2.53732000	0.13842000
H	-1.79588500	1.17672200	-1.98406700

H	2.14016500	0.98669800	2.31554600
H	1.54234300	-2.89847700	0.61338300
H	3.96527500	-3.04688300	0.10950400
O	5.76057000	-1.22596800	0.68068800
H	4.56248600	0.83767900	1.79875200
C	6.24462600	-0.74427700	-0.47237600
F	6.06558800	0.58457100	-0.60677300
F	5.68118600	-1.31535600	-1.55870700
F	7.55398900	-0.98998300	-0.51114100
C	-6.71474800	-0.37154700	-0.91868700
F	-6.60664300	0.18603100	-2.14000400
F	-7.89624100	-0.02345500	-0.40746200
F	-6.71740800	-1.70618500	-1.10527200

Table S11. DFT calculation result of *P*-**2b**

C	-0.02314300	-2.04952200	2.03621600
C	1.12073600	-2.46474000	2.73958800
C	2.20947600	-1.64361200	2.86513400
C	2.14606400	-0.33639500	2.34848300
C	1.03773100	0.11955700	1.62896000
C	-0.03416200	-0.79392500	1.36713100
C	-1.19669100	-0.49388500	0.53737800
C	-2.39393300	-1.17166500	0.80339600
C	-2.36186500	-2.38406900	1.55568000
C	-1.19710300	-2.85241000	2.06581500
C	-1.19669700	0.49385900	-0.53739400
C	-2.39395100	1.17161300	-0.80342600
C	-3.65944600	0.62108700	-0.33594300
C	-3.65943700	-0.62115000	0.33592400
C	-0.03416400	0.79392200	-1.36713400
C	-0.02316600	2.04951400	-2.03622800
C	-1.19714700	2.85236900	-2.06585600
C	-2.36190400	2.38400600	-1.55572900
C	-4.89687700	1.23076000	-0.63158000
C	-6.09302200	0.62599800	-0.31325300
C	-6.09301200	-0.62607900	0.31327100
C	-4.89685900	-1.23083200	0.63158200
C	1.03775100	-0.11953800	-1.62894700
C	2.14608200	0.33643400	-2.34846200
C	2.20947200	1.64365100	-2.86511400

C	1.12071300	2.46475500	-2.73958700
O	3.14582800	0.56259200	2.57786500
C	4.19424000	0.22799700	3.46540000
O	3.14587000	-0.56252900	-2.57782900
C	4.19428200	-0.22790800	-3.46535500
C	-0.26808600	-3.67345300	-1.71446800
C	0.77232100	-4.34566000	-1.10192200
C	1.89487900	-3.69340700	-0.62712400
C	1.96998000	-2.31372300	-0.77054900
C	0.94092000	-1.58855400	-1.37732300
C	-0.17068900	-2.29303000	-1.85150900
C	-0.17074100	2.29303300	1.85152100
C	0.94087600	1.58857100	1.37733300
C	1.96992400	2.31375200	0.77055400
C	1.89480000	3.69343500	0.62711900
C	0.77223100	4.34567200	1.10191300
C	-0.26816100	3.67345300	1.71446900
H	1.12216700	-3.44631200	3.20383800
H	3.07943700	-1.98050000	3.41308600
H	-3.26432500	-2.96574100	1.68489000
H	-1.15945300	-3.81126600	2.57389200
H	-1.15951600	3.81121700	-2.57395000
H	-3.26437700	2.96565000	-1.68496800
H	-4.92394500	2.18840000	-1.13447800
H	-7.02970900	1.11652700	-0.55731800
H	-7.02969300	-1.11661300	0.55735400
H	-4.92391100	-2.18846800	1.13448700
H	3.07943400	1.98055500	-3.41305600
H	1.12212600	3.44632500	-3.20384300
H	3.81098300	-0.04102300	4.45605800
H	4.80920100	-0.59147100	3.07591200
H	4.80777500	1.12498700	3.54859500
H	4.80784000	-1.12488200	-3.54854400
H	3.81102700	0.04110100	-4.45601700
H	4.80921800	0.59157600	-3.07586200
H	-1.12919400	-4.22213400	-2.07827000
H	2.68748500	-4.25905100	-0.15072200
H	2.84241400	-1.79197000	-0.39865400
H	-0.97437300	-1.75375800	-2.34160400
H	-0.97441500	1.75375300	2.34162300
H	2.84236600	1.79201200	0.39866200

H	2.68739600	4.25908800	0.15071200
F	0.68974500	5.69322400	0.96145500
H	-1.12927700	4.22212200	2.07827100
F	0.68985600	-5.69321400	-0.96147400

Table S12. DFT calculation result of *P*-**2c**

C	-0.01560600	2.44801600	1.53227600
C	-1.16131300	3.00905200	2.12186100
C	-2.25203600	2.23675600	2.42019500
C	-2.18878700	0.84757400	2.20542600
C	-1.07773000	0.24277800	1.61076400
C	-0.00480300	1.07606000	1.15635100
C	1.15883600	0.59986900	0.41542600
C	2.35638200	1.31861000	0.52851600
C	2.32507800	2.66602000	0.99780300
C	1.16000500	3.23589100	1.38994400
C	1.15882400	-0.59986300	-0.41542700
C	2.35635700	-1.31862300	-0.52852400
C	3.62186900	-0.67880900	-0.19439100
C	3.62188200	0.67877500	0.19437700
C	-0.00483300	-1.07604500	-1.15633200
C	-0.01566200	-2.44800800	-1.53223400
C	1.15994200	-3.23589500	-1.38991800
C	2.32502900	-2.66603500	-0.99780400
C	4.85971900	-1.33700700	-0.35420800
C	6.05599900	-0.67841900	-0.17290700
C	6.05601100	0.67833900	0.17290200
C	4.85974300	1.33694900	0.35420100
C	-1.07775600	-0.24275600	-1.61074500
C	-2.18883400	-0.84755000	-2.20537000
C	-2.25210900	-2.23673600	-2.42010600
C	-1.16139000	-3.00904100	-2.12178100
O	-3.19120200	0.02312000	2.62544100
C	-4.24272600	0.54906200	3.40909100
O	-3.19124500	-0.02309400	-2.62539200
C	-4.24279700	-0.54904800	-3.40899500
C	0.21809900	3.18839200	-2.53742100
C	-0.80674800	4.02252800	-2.10208800
C	-1.91475400	3.46836100	-1.46812500
C	-1.99834400	2.09528100	-1.27283400

C	-0.97691800	1.24529000	-1.70440600
C	0.13011800	1.81418300	-2.34315000
C	0.13013200	-1.81420600	2.34306000
C	-0.97691700	-1.24527200	1.70437600
C	-1.99837500	-2.09523000	1.27281300
C	-1.91480400	-3.46831800	1.46805700
C	-0.80678400	-4.02252600	2.10196200
C	0.21809400	-3.18842300	2.53728500
H	-1.16296800	4.06883200	2.35836500
H	-3.12399700	2.68717500	2.87561700
H	3.22854500	3.26028300	0.99838500
H	1.12273200	4.28259500	1.67650700
H	1.12265000	-4.28260100	-1.67646900
H	3.22848900	-3.26030900	-0.99840000
H	4.88651200	-2.37968800	-0.64177100
H	6.99267700	-1.20966700	-0.30749000
H	6.99269900	1.20956900	0.30749100
H	4.88655400	2.37962800	0.64177000
H	-3.12408600	-2.68715200	-2.87550100
H	-1.16306300	-4.06882500	-2.35826500
H	-3.86424100	1.03328300	4.31644400
H	-4.85415600	1.26122900	2.84275400
H	-4.85886200	-0.30575900	3.68804000
H	-3.86434300	-1.03330200	-4.31634400
H	-4.85421800	-1.26119000	-2.84261800
H	-4.85893100	0.30577100	-3.68795400
H	1.08766200	3.60515800	-3.03612100
H	-0.74271800	5.09524600	-2.25669000
H	-2.72000500	4.10836000	-1.12036600
H	-2.86515000	1.67594700	-0.77751600
H	0.92777700	1.16969800	-2.69854700
H	0.92781700	-1.16974700	2.69844800
H	-2.86519100	-1.67586300	0.77754000
H	-2.72007900	-4.10829100	1.12030700
H	-0.74276900	-5.09525000	2.25652700
H	1.08766700	-3.60522100	3.03594100

Table S13. DFT calculation result of *P*-**2d**

C	0.01244100	2.00138700	2.08020100
C	-1.13515900	2.40237100	2.78509200

C	-2.22630800	1.58049700	2.88273600
C	-2.16067600	0.28450100	2.33887300
C	-1.04634300	-0.15908700	1.62071700
C	0.02500600	0.76140600	1.38314800
C	1.18955100	0.48022600	0.54950800
C	2.38681800	1.14987300	0.83420100
C	2.35457100	2.34213000	1.61824700
C	1.18868900	2.79953200	2.13572900
C	1.18956200	-0.48019900	-0.54946300
C	2.38684600	-1.14981000	-0.83416800
C	3.65220700	-0.61152900	-0.35309300
C	3.65219200	0.61161700	0.35313100
C	0.02501700	-0.76141000	-1.38309200
C	0.01248400	-2.00138100	-2.08016300
C	1.18875900	-2.79948500	-2.13571500
C	2.35463000	-2.34205700	-1.61823200
C	4.88999900	-1.21216200	-0.66586000
C	6.08635000	-0.61682300	-0.33097600
C	6.08633500	0.61695500	0.33103600
C	4.88997100	1.21227300	0.66591000
C	-1.04636800	0.15905100	-1.62062900
C	-2.16070800	-0.28457600	-2.33875500
C	-2.22629500	-1.58056100	-2.88264800
C	-1.13511000	-2.40239100	-2.78504700
O	-3.16386700	-0.61732000	2.54266800
C	-4.22354900	-0.29407500	3.41903300
O	-3.16395500	0.61719600	-2.54249200
C	-4.22364400	0.29391700	-3.41883600
C	0.26867700	3.70574500	-1.68008000
C	-0.74506600	4.43700500	-1.05881300
C	-1.85679800	3.73612600	-0.59287500
C	-1.95411000	2.35722400	-0.73571300
C	-0.93887500	1.62418200	-1.35141200
C	0.17308200	2.32802900	-1.82654500
C	0.17312400	-2.32804400	1.82656500
C	-0.93881800	-1.62421200	1.35147200
C	-1.95408400	-2.35726400	0.73576100
C	-1.85675300	-3.73612500	0.59286000
C	-0.74494100	-4.43700800	1.05870300
C	0.26874900	-3.70578100	1.68002100
H	-1.13855800	3.37281300	3.27232300

H	-3.10032800	1.90711400	3.43050300
H	3.25803500	2.91789000	1.76618600
H	1.15168300	3.74385600	2.67078800
H	1.15178600	-3.74379900	-2.67079500
H	3.25811000	-2.91778700	-1.76618500
H	4.91678600	-2.15511500	-1.19587100
H	7.02302600	-1.10026800	-0.58912400
H	7.02300000	1.10041600	0.58919400
H	4.91673600	2.15522400	1.19592500
H	-3.10031400	-1.90720100	-3.43040300
H	-1.13847900	-3.37281900	-3.27230900
H	-3.85552500	-0.04354700	4.42055300
H	-4.82981800	0.53469600	3.03497700
H	-4.84196800	-1.18984400	3.47736900
H	-4.84211300	1.18965300	-3.47712700
H	-3.85563500	0.04343700	-4.42037300
H	-4.82985600	-0.53489800	-3.03478500
H	1.14545400	4.22163500	-2.06297800
H	-1.59799800	6.38176800	-0.66518900
H	-2.66426400	4.27720200	-0.10642400
H	-2.83119100	1.84405600	-0.36149700
H	0.97090300	1.78855600	-2.32710700
H	0.97092100	-1.78859400	2.32719000
H	-2.83119900	-1.84408900	0.36163600
H	-2.66424900	-4.27720800	0.10645700
C	-0.62681600	-5.92857900	0.88071200
H	1.14551500	-4.22167900	2.06292200
H	-0.22338100	6.40682100	-1.77870300
H	0.04529700	6.17494200	-0.05178200
H	0.03900700	-6.17427200	0.04560600
H	-1.59898700	-6.38277400	0.67232700
H	-0.21535500	-6.40611600	1.77472100
C	-0.62705000	5.92866400	-0.88145000

Table S14. DFT calculation result of *P*-**2e**

C	-1.86473700	-0.34873100	2.20130400
C	-1.98855700	-1.54882000	2.92184900
C	-0.95668500	-2.44748400	2.97632200
C	0.27048800	-2.12222800	2.37017500
C	0.44243600	-0.94628000	1.63341500

C	-0.68915500	-0.08835400	1.44372900
C	-0.69362800	1.10333200	0.60078900
C	-1.57864500	2.14083500	0.92243600
C	-2.69826000	1.87182800	1.76620400
C	-2.88218600	0.64059400	2.30149900
C	0.19166600	1.29156700	-0.54401300
C	0.58817800	2.59827300	-0.85708600
C	-0.17428900	3.73052300	-0.34798500
C	-1.33457300	3.48604300	0.41921800
C	0.66548100	0.20308500	-1.39389000
C	1.84791300	0.44029600	-2.14904700
C	2.38652700	1.75427000	-2.23676200
C	1.72493000	2.80524200	-1.69536200
C	0.14361100	5.06230900	-0.68876500
C	-0.66595700	6.11451900	-0.32085600
C	-1.83773400	5.86783700	0.40465000
C	-2.15829200	4.57774800	0.76644900
C	-0.02784200	-1.03397200	-1.59459500
C	0.59756200	-2.03621700	-2.34201300
C	1.85238600	-1.83969500	-2.94678600
C	2.43978300	-0.60400100	-2.87934300
O	1.36638800	-2.92067400	2.52684000
C	1.31251900	-4.00547500	3.43034700
O	-0.09319800	-3.20101300	-2.51131200
C	0.39101200	-4.17149400	-3.41617600
C	-3.77480700	-0.47613100	-1.43913600
C	-4.21483600	-1.62098900	-0.78112800
C	-3.28497200	-2.57407300	-0.36162900
C	-1.93587300	-2.37914700	-0.59357700
C	-1.46557100	-1.23206000	-1.24576900
C	-2.41075900	-0.29840000	-1.66595000
C	2.32214500	0.70180400	1.71152000
C	1.83766500	-0.54425100	1.28774200
C	2.73308100	-1.39634300	0.64692000
C	4.05905500	-1.03403600	0.42124700
C	4.51398200	0.21152200	0.84548100
C	3.63520700	1.08070700	1.49352600
H	-2.91382500	-1.74772100	3.45408600
H	-1.07101800	-3.36617600	3.53626800
H	-3.43685200	2.64070600	1.94803000
H	-3.77103800	0.41470100	2.88305500

H	3.29443100	1.90750600	-2.81244400
H	2.09855800	3.80591900	-1.86413600
H	1.03313000	5.27674000	-1.26622300
H	-0.39795000	7.12804500	-0.60129000
H	-2.48803700	6.68816800	0.69089000
H	-3.05794300	4.41608900	1.34550900
H	2.32179700	-2.63006100	-3.51764000
H	3.36506000	-0.41048100	-3.41386700
H	1.03893100	-3.67546800	4.43897900
H	0.61037300	-4.77826500	3.09623000
H	2.31887000	-4.42406200	3.44975500
H	0.51458900	-3.75627200	-4.42292900
H	1.34147300	-4.60235300	-3.07998200
H	-0.36567400	-4.95573300	-3.44121900
H	-4.46955400	0.28037800	-1.78148600
O	-5.52222900	-1.89664700	-0.50168900
H	-3.64334300	-3.45983900	0.15162200
H	-1.22973400	-3.12781900	-0.25702300
H	-2.08215000	0.59346300	-2.18989400
H	1.65582700	1.38432500	2.22913300
H	2.39463900	-2.36738800	0.30804500
H	4.71511900	-1.72873300	-0.08814200
O	5.78973100	0.66691600	0.67607400
H	4.00345900	2.04585400	1.82374400
C	6.72814000	-0.18662100	0.05625300
H	6.43210400	-0.43113500	-0.97096400
H	6.86132600	-1.11517600	0.62400100
H	7.66972100	0.36215300	0.03769600
C	-6.50390700	-0.96978400	-0.91725400
H	-7.46189600	-1.38208800	-0.60055700
H	-6.50448000	-0.84915700	-2.00700800
H	-6.35645800	0.00872500	-0.44525100

Table S15. DFT calculation result of *P*-**2f**

C	-1.93998700	0.05779400	2.14239300
C	-2.31713000	-1.08548800	2.86819400
C	-1.49137200	-2.17470800	2.95059300
C	-0.21423900	-2.11339600	2.36297700
C	0.20236900	-1.00588400	1.61890500
C	-0.72192700	0.06817000	1.40744500

C	-0.46552300	1.22974400	0.56232500
C	-1.12854600	2.42713800	0.86310500
C	-2.30028200	2.39533800	1.67686800
C	-2.74110500	1.23107200	2.21224100
C	0.46551100	1.22974400	-0.56233900
C	1.12852300	2.42714100	-0.86313000
C	0.60293300	3.69266600	-0.36749800
C	-0.60295200	3.69266400	0.36748000
C	0.72192400	0.06816300	-1.40744700
C	1.93997900	0.05779300	-2.14240200
C	2.74108100	1.23108100	-2.21227200
C	2.30025000	2.39534700	-1.67690600
C	1.19641600	4.93001500	-0.69455400
C	0.60890900	6.12614800	-0.34534900
C	-0.60891800	6.12614700	0.34536100
C	-1.19643000	4.93001300	0.69455200
C	-0.20236300	-1.00590100	-1.61889600
C	0.21425200	-2.11341300	-2.36296400
C	1.49138400	-2.17472000	-2.95058300
C	2.31713100	-1.08549200	-2.86819500
O	0.69470600	-3.11373600	2.54309100
C	0.40929600	-4.16058300	3.44987600
O	-0.69468600	-3.11376100	-2.54307400
C	-0.40926200	-4.16061400	-3.44984600
C	-3.75555700	0.29629200	-1.49460200
C	-4.40882700	-0.74164100	-0.84577200
C	-3.71351500	-1.86496000	-0.42015000
C	-2.34532500	-1.94177500	-0.64362400
C	-1.65500500	-0.91179600	-1.28674800
C	-2.38644700	0.20062500	-1.71384000
C	2.38645700	0.20063600	1.71386200
C	1.65501000	-0.91177500	1.28675400
C	2.34532600	-1.94174700	0.64361400
C	3.71351600	-1.86493200	0.42013700
C	4.40883200	-0.74162100	0.84577400
C	3.75556700	0.29630300	1.49462300
H	-3.27271600	-1.08609300	3.38374200
H	-1.79892400	-3.04386700	3.51676400
H	-2.87508500	3.29763100	1.83452600
H	-3.67269300	1.19348600	2.76859500
H	3.67266100	1.19350200	-2.76863900

H	2.87503700	3.29764700	-1.83458600
H	2.12636900	4.95701400	-1.24692600
H	1.08606800	7.06282400	-0.61460800
H	-1.08607100	7.06282200	0.61463200
H	-2.12637900	4.95700900	1.24693100
H	1.79894000	-3.04387900	-3.51674900
H	3.27271500	-1.08609000	-3.38374800
H	0.19540100	-3.77513600	4.45296800
H	-0.43050700	-4.77588400	3.10719000
H	1.30944000	-4.77409100	3.48456300
H	-0.19536800	-3.77517700	-4.45294200
H	0.43054700	-4.77590200	-3.10715000
H	-1.30940000	-4.77413200	-3.48452900
H	-4.30912100	1.16636600	-1.82833200
H	-4.23574800	-2.66847900	0.08650100
H	-1.80531700	-2.81673500	-0.30511900
H	-1.87823500	1.00747500	-2.23126500
H	1.87824900	1.00747900	2.23130300
H	1.80531500	-2.81670000	0.30509800
H	4.23574500	-2.66844500	-0.08652700
Cl	6.13314300	-0.63312500	0.55939400
H	4.30913400	1.16637000	1.82836600
Cl	-6.13313900	-0.63314300	-0.55939300

Table S16. DFT calculation result of *P*-**2g**

C	1.59850700	0.25020000	-2.40215400
C	1.88263500	-0.90977900	-3.14380300
C	1.07408600	-2.01216400	-3.06539300
C	-0.10878800	-1.94327400	-2.30568800
C	-0.43371600	-0.81409100	-1.54841500
C	0.50768300	0.26362600	-1.48986000
C	0.37363900	1.43298800	-0.62789500
C	0.97459100	2.63159000	-1.03526400
C	1.99024800	2.60283700	-2.03768400
C	2.35018300	1.43685300	-2.62718600
C	-0.37383900	1.43376900	0.62598500
C	-0.97494000	2.63283000	1.03178200
C	-0.53515400	3.89790600	0.45829000
C	0.53462700	3.89736800	-0.46345600
C	-0.50771300	0.26553100	1.48950000

C	-1.59853800	0.25316000	2.40180800
C	-2.35035800	1.44001500	2.62529500
C	-1.99056600	2.60527200	2.03426900
C	-1.06859200	5.13591000	0.87510800
C	-0.54591800	6.33178500	0.43455000
C	0.54505300	6.33127700	-0.44296100
C	1.06789200	5.13488800	-0.88192700
C	0.43379400	-0.81201300	1.54943200
C	0.10899500	-1.94025500	2.30815100
C	-1.07387200	-2.00829500	3.06795000
C	-1.88253500	-0.90589300	3.14495500
O	-1.02219500	-2.95605400	-2.32921400
C	-0.83870500	-4.03866300	-3.21895300
O	1.02252100	-2.95290100	2.33291600
C	0.83919300	-4.03445100	3.22397600
C	3.96036200	0.49861200	1.17146600
C	4.59666500	-0.52116900	0.46175800
C	3.83836300	-1.61427700	0.03808900
C	2.48475400	-1.69108900	0.33273800
C	1.84208500	-0.69185000	1.06725000
C	2.60947100	0.40415700	1.47636000
C	-2.48463900	-1.69158500	-0.33049400
C	-1.84203900	-0.69338000	-1.06647000
C	-2.60949200	0.40199400	-1.47714900
C	-3.96038200	0.49682000	-1.17236800
C	-4.59661500	-0.52195900	-0.46115900
C	-3.83824300	-1.61441300	-0.03592300
N	5.99052200	-0.45325200	0.19252400
N	-5.99045000	-0.45369400	-0.19191500
C	-6.47959100	-0.80138800	1.08893600
C	-6.88732100	-0.08579200	-1.22414000
C	6.47978900	-0.80288200	-1.08775300
C	6.88729400	-0.08381000	1.22428100
C	-7.98265700	0.74119300	-0.95269400
C	-8.86339300	1.09645400	-1.96716600
C	-8.66063600	0.65024600	-3.27045500
C	-7.56578800	-0.16460300	-3.54512200
C	-6.68962000	-0.53812500	-2.53289300
C	-7.64723400	-1.55904400	1.23026400
C	-8.12113500	-1.89023100	2.49424000
C	-7.43503700	-1.48805700	3.63708200

C	-6.26784300	-0.74148500	3.49824000
C	-5.79553200	-0.39338000	2.23865300
C	7.64741800	-1.56078900	-1.22782500
C	8.12143700	-1.89388600	-2.49125600
C	7.43547600	-1.49339100	-3.63477000
C	6.26829600	-0.74656600	-3.49716500
C	5.79586400	-0.39656800	-2.23814900
C	7.98268800	0.74271900	0.95167600
C	8.86332500	1.09951900	1.96569300
C	8.66040900	0.65533500	3.26964900
C	7.56550100	-0.15904700	3.54545700
C	6.68943200	-0.53410800	2.53371100
H	2.75041300	-0.91765400	-3.79631300
H	1.31269400	-2.89725700	-3.64006400
H	2.51296800	3.51048200	-2.30628400
H	3.16487300	1.40936900	-3.34491800
H	-3.16504600	1.41336600	3.34306100
H	-2.51337900	3.51320600	2.30170600
H	-1.89955800	5.16359500	1.56736600
H	-0.97442800	7.26858400	0.77571200
H	0.97343100	7.26768100	-0.78537100
H	1.89884600	5.16176300	-1.57423100
H	-1.31239600	-2.89268400	3.64373500
H	-2.75032700	-0.91302900	3.79745600
H	-1.72376100	-4.66511900	-3.10779700
H	-0.76535200	-3.69734600	-4.25773800
H	0.05034400	-4.62700600	-2.96408800
H	1.72432400	-4.66093000	3.11355200
H	0.76583300	-3.69188200	4.26234800
H	-0.04978900	-4.62321700	2.96985500
H	4.53203900	1.35853100	1.50356500
H	4.31568000	-2.41194900	-0.52111200
H	1.92200700	-2.55434400	0.00063900
H	2.14208200	1.19768300	2.05061600
H	-1.92182700	-2.55429500	0.00290200
H	-2.14214800	1.19473200	-2.05253000
H	-4.53209900	1.35624500	-1.50567000
H	-4.31549500	-2.41128500	0.52447400
H	-8.13969400	1.10304500	0.05752200
H	-9.70760800	1.73914900	-1.73714100
H	-9.34587000	0.93554300	-4.06173200

H	-7.39475800	-0.52419200	-4.55510100
H	-5.84267300	-1.17872400	-2.75224500
H	-8.18177100	-1.88512300	0.34487100
H	-9.02912900	-2.47860800	2.58374500
H	-7.80534000	-1.75198800	4.62210300
H	-5.72641700	-0.41272600	4.38054000
H	-4.89198700	0.19583700	2.13228300
H	8.18185300	-1.88556300	-0.34189000
H	9.02941800	-2.48243000	-2.57978600
H	7.80587400	-1.75880500	-4.61935600
H	5.72697900	-0.41910000	-4.38001300
H	4.89233000	0.19283600	-2.13274800
H	8.13984900	1.10300100	-0.05908200
H	9.70758700	1.74182700	1.73476700
H	9.34556700	0.94183300	4.06055800
H	7.39434400	-0.51706100	4.55597400
H	5.84243100	-1.17432700	2.75396600

Table S17. DFT calculation result of *P*-**3a**

C	0.01992900	-2.78335900	0.56066300
C	0.17757000	-1.62472000	-0.21522100
C	-0.82058800	-1.28350800	-1.15306900
C	-2.02845400	-2.00493600	-1.14452800
C	-2.21873800	-3.11974500	-0.31707200
C	-1.16196300	-3.50243700	0.50775400
C	1.21146200	-3.27249400	1.33368300
C	2.44957900	-3.12701900	0.44693300
C	2.63072000	-1.67093900	0.08127600
C	1.46663000	-0.88534400	-0.07342200
C	3.88538300	-1.07283800	-0.01711100
C	3.99088900	0.30345700	-0.26989700
C	2.85095200	1.09818500	-0.31382400
C	1.58299200	0.51737000	-0.09077800
C	2.90019200	2.55984600	-0.70313700
C	1.65253800	2.90778600	-1.51643500
C	0.44677100	2.63448500	-0.66374200
C	0.44697000	1.46386900	0.11082400
C	-0.60839300	3.52814100	-0.58247500
C	-1.68511500	3.31644000	0.27789900
C	-1.62113800	2.20712500	1.13119600

C	-0.55192300	1.29587400	1.09394300
O	-3.00007900	-1.65825600	-2.05655500
C	-4.14532200	-1.01352400	-1.51395400
O	-2.62885200	2.01339300	2.05089700
C	-2.48255300	2.74487800	3.26441600
C	5.11836600	-1.90561300	0.10927400
C	5.33735200	0.89291900	-0.55319800
O	6.04813500	-1.31143900	0.87722800
C	7.31617700	-1.97340300	0.93630000
O	5.63000700	1.91570300	0.26354200
C	6.89819000	2.54171800	0.04134600
O	5.27792900	-2.99423300	-0.39399700
O	6.08177800	0.51042000	-1.42790400
C	-3.45063900	-3.95362700	-0.35407300
C	-2.81661800	4.28081900	0.30589900
C	-3.98536300	-4.41389300	-1.56274200
C	-5.10681600	-5.23515500	-1.57282400
C	-5.71784600	-5.60920500	-0.37827900
C	-5.19536300	-5.15743700	0.82913100
C	-4.07029200	-4.33845500	0.83922300
C	-2.56791100	5.65755200	0.28456800
C	-3.61472100	6.57383400	0.26678600
C	-4.93247200	6.12829900	0.26912300
C	-5.19307600	4.76045900	0.29232700
C	-4.14684100	3.84555000	0.31398600
C	-0.56337300	-0.35537200	-2.29665200
C	-1.39412000	0.71891700	-2.61827500
C	-1.16932800	1.47841600	-3.76076800
C	-0.10805000	1.17562200	-4.60908700
C	0.73304600	0.11152300	-4.29820800
C	0.50517400	-0.64432700	-3.15309000
C	-0.43382200	0.31667400	2.21583600
C	0.70834800	0.34540300	3.02398500
C	0.80978200	-0.46497900	4.15026800
C	-0.23325000	-1.32246200	4.48711800
C	-1.37030800	-1.36608700	3.68464100
C	-1.47059000	-0.55318400	2.56151900
H	-1.25659300	-4.41103900	1.09509400
H	1.34668600	-2.69054700	2.25330500
H	1.06658400	-4.31663200	1.62446500
H	2.33245500	-3.73732000	-0.45690900

H	3.33679900	-3.50364200	0.95508400
H	2.95189700	3.19809600	0.18782800
H	3.79910600	2.76219500	-1.28797600
H	1.66843600	3.95831000	-1.81978400
H	1.62812000	2.30153200	-2.42979500
H	-0.60934700	4.40273600	-1.22630800
H	-4.76698300	-0.72588100	-2.36283200
H	-4.71169500	-1.68348100	-0.85972000
H	-3.85969600	-0.11759500	-0.95049400
H	-3.35472200	2.50938400	3.87514600
H	-1.57373800	2.43861900	3.79345900
H	-2.45392100	3.82252700	3.07066700
H	7.92493700	-1.37992800	1.61643900
H	7.19845000	-2.99110400	1.31190400
H	7.76541500	-2.00426500	-0.05843700
H	6.96499200	3.33822300	0.78038600
H	7.70529300	1.81977600	0.17853700
H	6.95251100	2.94723700	-0.97100500
H	-3.51644400	-4.12219500	-2.49541000
H	-5.50364200	-5.58806700	-2.51967400
H	-6.59445500	-6.24910700	-0.38958500
H	-5.66446300	-5.43974100	1.76652900
H	-3.67123900	-3.98203700	1.78413500
H	-1.54268300	6.01441900	0.29807500
H	-3.39843600	7.63755400	0.25646800
H	-5.75100500	6.84087500	0.25497500
H	-6.21796000	4.40251800	0.29250000
H	-4.35712500	2.78281300	0.34049000
H	-2.21691400	0.97702200	-1.96269900
H	-1.82855100	2.31057500	-3.98772700
H	0.06118000	1.76394600	-5.50557900
H	1.56418900	-0.13882700	-4.94994800
H	1.15540500	-1.48360300	-2.92768200
H	1.51945500	1.02224400	2.77455200
H	1.70195400	-0.41934200	4.76702200
H	-0.16112100	-1.95207600	5.36850900
H	-2.18729300	-2.03549900	3.93585200
H	-2.36135300	-0.58996300	1.94611600

Table S19. DFT calculation result of *P*-**3b**

C	0.48307300	-2.78151500	0.66841700
C	0.65461900	-1.65295400	-0.14770700
C	-0.35384600	-1.31688600	-1.07626300
C	-1.57988700	-2.00426800	-1.01829100
C	-1.78306800	-3.08699100	-0.15155500
C	-0.71752400	-3.47089900	0.66194400
C	1.67747500	-3.27702200	1.43315900
C	2.90113400	-3.19027600	0.51898500
C	3.11117100	-1.75095700	0.10554600
C	1.96372200	-0.94207500	-0.05388400
C	4.37799200	-1.18723100	-0.03162400
C	4.51238400	0.17807800	-0.32742600
C	3.39134000	0.99875600	-0.37726000
C	2.11351200	0.45619900	-0.11656800
C	3.46851500	2.44671600	-0.81057900
C	2.21731300	2.79980600	-1.61629400
C	1.01809600	2.58104300	-0.73865600
C	1.00389000	1.43570600	0.07244200
C	-0.01703600	3.49918700	-0.67345400
C	-1.08700000	3.34025900	0.20699100
C	-1.03192900	2.25860700	1.09661900
C	0.01603100	1.32282700	1.07453800
O	-2.56273700	-1.65876200	-1.92025800
C	-3.67136600	-0.95820600	-1.37138500
O	-2.02845700	2.11811000	2.03918400
C	-1.84514100	2.89079500	3.22150000
C	5.59244900	-2.04567300	0.10053700
C	5.86786300	0.72585100	-0.64821600
O	6.54823000	-1.45228800	0.83684500
C	7.80061000	-2.14304500	0.89655200
O	6.19787900	1.76408900	0.13422000
C	7.47715000	2.35202200	-0.12466100
O	5.71856600	-3.15207200	-0.37269700
O	6.58956300	0.30046800	-1.52224600
C	-3.03869000	-3.88285000	-0.13080000
C	-2.19813200	4.32624600	0.21558800
C	-3.63450400	-4.35279300	-1.30097900
C	-4.78222000	-5.14193600	-1.26796700
C	-5.35916600	-5.47281800	-0.04248900
C	-4.77779000	-5.01024900	1.13974500
C	-3.63430700	-4.23076000	1.08963700

C	-1.93217700	5.69993300	0.11872100
C	-2.95370900	6.63348800	0.08030500
C	-4.28497400	6.21528100	0.13434900
C	-4.57418800	4.85510900	0.23327600
C	-3.53399500	3.92933500	0.27615100
C	-0.09562300	-0.43392100	-2.25484200
C	-0.90216400	0.65303800	-2.59486800
C	-0.67918700	1.36953700	-3.76516600
C	0.35596900	1.01016300	-4.62358900
C	1.17301800	-0.06721100	-4.29489900
C	0.94701000	-0.77990400	-3.12207800
C	0.13123900	0.37912300	2.22682500
C	1.28985400	0.40529900	3.01143500
C	1.39437100	-0.36999200	4.16182900
C	0.33773500	-1.18941300	4.54743000
C	-0.81625300	-1.23024300	3.76932600
C	-0.91941600	-0.45229500	2.62194500
H	-0.82199500	-4.35824100	1.27945100
H	1.84575100	-2.67099600	2.33154200
H	1.51250000	-4.30780100	1.75890900
H	2.75066400	-3.82430600	-0.36336200
H	3.78853000	-3.57405800	1.02144600
H	3.54709400	3.10928300	0.06046900
H	4.36340500	2.61125900	-1.41323100
H	2.25328800	3.84016700	-1.95137800
H	2.16547800	2.16737400	-2.51066400
H	-0.00807200	4.35074600	-1.34747400
H	-4.24308800	-1.58817100	-0.68284800
H	-3.34170800	-0.05593200	-0.84320100
H	-4.30390200	-0.67486000	-2.21386200
H	-2.70937300	2.69495800	3.85719700
H	-0.93218700	2.58645700	3.74456400
H	-1.79982300	3.95971200	2.98678500
H	8.23267100	-2.21571700	-0.10361800
H	8.43466100	-1.54408700	1.54821600
H	7.66467100	-3.14551600	1.30556900
H	8.26845600	1.61409700	0.01949000
H	7.52503600	2.72883200	-1.14839700
H	7.57549000	3.16622100	0.59123000
H	-3.19649900	-4.09759600	-2.25907500
H	-5.20799200	-5.49184200	-2.20002200

O	-6.47967200	-6.23287000	0.10148200
H	-5.24080100	-5.27203200	2.08488500
H	-3.19712700	-3.87196000	2.01657200
H	-0.90293700	6.04401700	0.08994800
H	-2.74402800	7.69544600	0.01393700
O	-5.22229300	7.20124800	0.08856900
H	-5.59672200	4.50147500	0.27563600
H	-3.77148900	2.87540700	0.36090500
H	-1.70315000	0.95616000	-1.93162300
H	-1.31873600	2.21329500	-4.00528800
H	0.52394600	1.56532500	-5.54124200
H	1.98397900	-0.36130200	-4.95378500
H	1.57815300	-1.62970000	-2.88223600
H	2.11202200	1.05313900	2.72416100
H	2.29986100	-0.32662100	4.75905200
H	0.41237800	-1.79162100	5.44758100
H	-1.64411600	-1.87036800	4.05847900
H	-1.82312100	-0.48689000	2.02569500
C	-6.58722700	6.83599700	0.14284100
H	-7.14989400	7.76773300	0.09319400
H	-6.82506000	6.31826000	1.07926700
H	-6.86429900	6.19974600	-0.70562200
C	-7.10776500	-6.73347700	-1.06223900
H	-7.44928300	-5.92034800	-1.71321900
H	-7.96910800	-7.30449300	-0.71686800
H	-6.43766800	-7.39325400	-1.62531500

Table S20. DFT calculation result of *P*-**3c**

C	0.23345000	-2.78959200	0.60193400
C	0.40207900	-1.64294500	-0.18945200
C	-0.59343700	-1.30381500	-1.13088300
C	-1.80929100	-2.01125900	-1.10976400
C	-2.00977500	-3.11325800	-0.26790700
C	-0.95556100	-3.49754400	0.55943100
C	1.42120600	-3.28136000	1.37905700
C	2.65896400	-3.16155400	0.48796800
C	2.85513000	-1.71262100	0.10221500
C	1.69967100	-0.91629900	-0.06045800
C	4.11614600	-1.12988700	-0.00770300
C	4.23634400	0.24134800	-0.27967800

C	3.10519600	1.04818600	-0.33199500
C	1.83158400	0.48463100	-0.09822500
C	3.16972200	2.50369800	-0.74140300
C	1.92433200	2.85394600	-1.55725100
C	0.71738100	2.60588800	-0.69849900
C	0.70659500	1.44637800	0.09270700
C	-0.32811200	3.51176700	-0.62834300
C	-1.40387800	3.32474900	0.23890100
C	-1.34949100	2.22774000	1.10842000
C	-0.29129400	1.30343200	1.08076800
O	-2.78039600	-1.66796800	-2.02424900
C	-3.91092800	-0.99181700	-1.48895500
O	-2.35789000	2.06089200	2.03308600
C	-2.19013100	2.79493000	3.24282500
C	5.34009800	-1.97515200	0.12617300
C	5.58872700	0.81196900	-0.57424100
O	6.27876000	-1.38169600	0.88318800
C	7.53932700	-2.05782900	0.94811200
O	5.89525400	1.84105100	0.22897200
C	7.17051400	2.44929700	-0.00360300
O	5.48468900	-3.07207700	-0.36323800
O	6.32538900	0.40996600	-1.44663100
C	-3.25181000	-3.93169200	-0.29321100
C	-2.52496400	4.30083000	0.25823000
C	-3.79874100	-4.39389200	-1.49631100
C	-4.92997000	-5.20082300	-1.50562700
C	-5.51211500	-5.53980000	-0.29637000
C	-5.00650400	-5.10637500	0.91482400
C	-3.87134100	-4.30161000	0.90477800
C	-2.26446200	5.67464600	0.20939500
C	-3.29608900	6.60757800	0.18238300
C	-4.59859200	6.14532400	0.20458800
C	-4.90371800	4.79634800	0.25553200
C	-3.86000200	3.87957600	0.28515700
C	-0.32665200	-0.39616600	-2.28871200
C	-1.14354000	0.68397200	-2.62561500
C	-0.91063400	1.42281900	-3.78000700
C	0.14521300	1.09307900	-4.62496400
C	0.97264400	0.02283600	-4.29895100
C	0.73663000	-0.71236800	-3.14215700
C	-0.18196600	0.33789500	2.21536800

C	0.96301300	0.36287200	3.01967800
C	1.05722200	-0.43306800	4.15678600
C	0.00405800	-1.27195200	4.50861000
C	-1.13591700	-1.31184500	3.71010800
C	-1.22894900	-0.51346700	2.57598500
H	-1.05732400	-4.39860000	1.15718800
H	1.56471500	-2.68823900	2.29019600
H	1.26563200	-4.31971600	1.68456700
H	2.53384800	-3.78305600	-0.40711300
H	3.54293300	-3.54076800	0.99976800
H	3.23036800	3.15360800	0.14051200
H	4.06951900	2.68818900	-1.33071600
H	1.95120600	3.89980400	-1.87551400
H	1.89139000	2.23520200	-2.46192400
H	-0.32131600	4.37559700	-1.28660600
H	-3.60620800	-0.09125800	-0.94340100
H	-4.53163500	-0.70873400	-2.34001400
H	-4.48608800	-1.63863300	-0.81906200
H	-3.06432500	2.58140400	3.85861900
H	-1.28578500	2.47204700	3.76920200
H	-2.13876700	3.87074900	3.04324700
H	8.15712900	-1.46169100	1.61762600
H	7.41061100	-3.06838000	1.33903400
H	7.98482200	-2.10852900	-0.04745200
H	7.22707800	2.84206800	-1.02081300
H	7.24859100	3.25356500	0.72581100
H	7.96908000	1.71927200	0.14033900
H	-3.33254600	-4.11499300	-2.43384100
H	-5.35747000	-5.56954000	-2.43113100
F	-6.61639600	-6.32336400	-0.30045000
H	-5.49589100	-5.39242400	1.83878300
H	-3.46569800	-3.94549500	1.84645300
H	-1.23711900	6.02423900	0.20816800
H	-3.10100900	7.67340600	0.15145100
F	-5.61137500	7.04318100	0.17900500
H	-5.94012600	4.47874700	0.26951100
H	-4.08236500	2.82049100	0.33358700
H	-1.96176700	0.96325000	-1.97299700
H	-1.55938900	2.25974500	-4.01925200
H	0.32060200	1.66510200	-5.53072700
H	1.79927500	-0.24849000	-4.94797000

H	1.37620500	-1.55660100	-2.90506000
H	1.78211000	1.02559500	2.75878300
H	1.95164000	-0.39045300	4.77043000
H	0.07046100	-1.88976500	5.39871400
H	-1.96103400	-1.96632400	3.97382600
H	-2.12214600	-0.54655500	1.96387000

Table S21. DFT calculation result of *P*-**3d**

C	0.25175400	-2.79186400	0.59050900
C	0.41898800	-1.64254200	-0.19706000
C	-0.57961700	-1.29961100	-1.13377700
C	-1.79545900	-2.00710400	-1.11251000
C	-1.99510400	-3.11205300	-0.27382600
C	-0.93807400	-3.49853700	0.54913600
C	1.44115600	-3.28675800	1.36327700
C	2.67723500	-3.16277500	0.47041800
C	2.87263700	-1.71204200	0.09106100
C	1.71628600	-0.91563900	-0.06709700
C	4.13321000	-1.12819400	-0.01638300
C	4.25245500	0.24479700	-0.28133200
C	3.12083500	1.05104800	-0.32886200
C	1.84738500	0.48559600	-0.09715900
C	3.18396500	2.50879200	-0.73065900
C	1.93812400	2.86259500	-1.54419500
C	0.73134000	2.60895900	-0.68672900
C	0.72179500	1.44557200	0.09844900
C	-0.31569500	3.51284400	-0.61296200
C	-1.39371100	3.31966900	0.25029100
C	-1.33759700	2.21820800	1.11456700
C	-0.27714900	1.29670200	1.08467700
O	-2.76793300	-1.65688400	-2.02272900
C	-3.90091400	-0.99208000	-1.47880200
O	-2.34492200	2.04287200	2.03884100
C	-2.19002800	2.78857000	3.24239100
C	5.35769700	-1.97259600	0.11403200
C	5.60417100	0.81742100	-0.57296700
O	6.29547500	-1.38173000	0.87505900
C	7.55670900	-2.05610700	0.93647400
O	5.90972700	1.84421800	0.23418600
C	7.18389600	2.45458900	0.00365400

O	5.50516400	-3.06699500	-0.38037200
O	6.34277700	0.41954300	-1.44579800
C	-3.23705300	-3.93025600	-0.29555700
C	-2.51705600	4.29271100	0.26844200
C	-3.79447000	-4.39077100	-1.49476500
C	-4.92313600	-5.19802900	-1.48793000
C	-5.54309500	-5.57421200	-0.29204200
C	-4.98759900	-5.11379400	0.89993400
C	-3.85229600	-4.30744700	0.89951100
C	-2.26552600	5.66619500	0.22382200
C	-3.30842100	6.58748100	0.19716300
C	-4.63834600	6.17065400	0.21029600
C	-4.88883900	4.79621300	0.25929500
C	-3.85265200	3.87332600	0.29105900
C	-0.31703900	-0.38546400	-2.28736000
C	-1.13619800	0.69575600	-2.61539500
C	-0.90705300	1.44213400	-3.76564700
C	0.14703300	1.11910700	-4.61546900
C	0.97658100	0.04782000	-4.29836800
C	0.74435600	-0.69489700	-3.14555000
C	-0.16567200	0.32788900	2.21624200
C	0.97906800	0.35361500	3.02089300
C	1.07617600	-0.44653700	4.15482800
C	0.02601900	-1.29063000	4.50315900
C	-1.11383300	-1.33118200	3.70447500
C	-1.20965900	-0.52855000	2.57358300
H	-1.03974500	-4.40084800	1.14491700
H	1.58651600	-2.69794700	2.27698700
H	1.28616600	-4.32658100	1.66420100
H	2.54961700	-3.77971400	-0.42749100
H	3.56239500	-3.54453600	0.97834800
H	3.24366200	3.15379600	0.15494100
H	4.08372500	2.69736500	-1.31881100
H	1.96409800	3.91033800	-1.85640100
H	1.90565100	2.24899800	-2.45243700
H	-0.30975600	4.38074300	-1.26578400
H	-4.47125100	-1.64854200	-0.81440100
H	-3.59987600	-0.09464800	-0.92582000
H	-4.52450300	-0.70423400	-2.32627200
H	-2.15454500	3.86344700	3.03484900
H	-3.06189300	2.56679100	3.85875800

H	-1.28175900	2.48262900	3.77267000
H	8.00318200	-2.09972100	-0.05904500
H	8.17326000	-1.46337900	1.61024300
H	7.42961000	-3.06947700	1.32067900
H	7.98355200	1.72506000	0.14434400
H	7.23989000	2.85156700	-1.01200100
H	7.26138100	3.25615700	0.73618100
H	-3.33561500	-4.11035700	-2.43596800
H	-5.33051100	-5.54848100	-2.43287600
C	-6.77105400	-6.44726900	-0.30290700
H	-5.44779100	-5.38627300	1.84576900
H	-3.44459100	-3.95697800	1.84309700
H	-1.23995000	6.02269600	0.22839200
H	-3.08036500	7.64955100	0.17185100
C	-5.77280900	7.16071200	0.15903400
H	-5.91623300	4.44152500	0.27292600
H	-4.07623600	2.81392200	0.33829200
H	-1.95278100	0.96999100	-1.95861800
H	-1.55704700	2.28028100	-3.99717700
H	0.31968700	1.69740600	-5.51783300
H	1.80206900	-0.21827900	-4.95107400
H	1.38544500	-1.53983300	-2.91511700
H	1.79581200	1.02019800	2.76240600
H	1.97065100	-0.40340200	4.76844000
H	0.09485500	-1.91228400	5.39046300
H	-1.93632300	-1.99043700	3.96444500
H	-2.10236200	-0.56303900	1.96091600
H	-6.53942700	6.92693700	0.90360400
H	-6.25902300	7.15155500	-0.82246000
H	-5.42147000	8.17852200	0.34473900
H	-7.59998700	-5.95904700	-0.82558100
H	-7.10473000	-6.67654600	0.71190200
H	-6.57805200	-7.39530700	-0.81483300

Table S23. DFT calculation result of *P*-**3e**

C	-2.62724700	2.45564000	-0.88187100
C	-1.52599800	2.53203100	-0.01507900
C	-1.39406000	1.57399700	1.01268800
C	-2.26746700	0.47091100	1.02551600
C	-3.32618600	0.35221700	0.11445700

C	-3.49464600	1.37890700	-0.81506300
C	-2.89461100	3.63642500	-1.77030000
C	-2.68409500	4.90985200	-0.94869800
C	-1.25829600	4.94992800	-0.44575700
C	-0.63032100	3.71685800	-0.15971800
C	-0.53112200	6.13430200	-0.34331300
C	0.81776800	6.09998200	0.04318600
C	1.46826700	4.88340900	0.21264300
C	0.76836500	3.67781500	-0.01436400
C	2.88299900	4.78964900	0.74201500
C	3.00959100	3.54767800	1.62670200
C	2.68518900	2.34388800	0.78909800
C	1.59494200	2.43793100	-0.08999300
C	3.49092600	1.21834100	0.78359700
C	3.27033900	0.15727400	-0.09503700
C	2.22425400	0.28840300	-1.01914500
C	1.41293200	1.43659800	-1.06709400
O	-2.13625600	-0.44982700	2.04270200
C	-1.61350100	-1.71507700	1.66550900
O	2.04675300	-0.67318500	-1.99018200
C	1.44769500	-1.88536000	-1.55548100
C	-1.20040100	7.44230900	-0.60756100
C	1.53057400	7.38437100	0.33196400
O	-0.42345900	8.26642600	-1.33157200
C	-0.92987900	9.59290000	-1.51375900
O	2.64520200	7.52579600	-0.39990700
C	3.39163600	8.72461400	-0.16546700
O	-2.31385500	7.74194400	-0.24031300
O	1.16395200	8.20276200	1.14531200
C	-4.31847200	-0.75383800	0.16299000
C	4.19780100	-1.00417400	-0.07838100
C	-4.71914800	-1.39531500	-1.01298400
C	-5.68973700	-2.38888700	-1.00419500
C	-6.28634700	-2.78375700	0.19589700
C	-5.88633700	-2.15251600	1.37899000
C	-4.92595300	-1.15187800	1.35949200
C	4.55194700	-1.60748900	1.13244500
C	5.45159200	-2.66439700	1.18095000
C	6.04766700	-3.13985300	0.01006000
C	5.70663900	-2.53613700	-1.20512400
C	4.79098100	-1.49492000	-1.24728600

N	-7.27367100	-3.79756700	0.21577500
N	6.97707500	-4.20635700	0.05282500
C	6.95108400	-5.21335000	-0.94502800
C	7.94159600	-4.26624100	1.09070500
C	-8.41208200	-3.66485900	1.05142500
C	-7.13845700	-4.93963000	-0.61332200
C	-5.90366800	-5.58370600	-0.73851100
C	-5.77377600	-6.69921600	-1.55722900
C	-6.87285900	-7.20095800	-2.24929800
C	-8.10534700	-6.56677000	-2.11881100
C	-8.23900800	-5.44057200	-1.31520700
C	-8.89084100	-4.76224600	1.77335200
C	-10.01233700	-4.63320500	2.58408000
C	-10.66288600	-3.40792400	2.70199800
C	-10.18256100	-2.31189200	1.99045500
C	-9.07207400	-2.43754500	1.16406400
C	8.14148400	-5.68973200	-1.50246600
C	8.11281200	-6.68368200	-2.47357600
C	6.90058800	-7.20605300	-2.91626200
C	5.71366000	-6.72754300	-2.36801700
C	5.73525600	-5.74600800	-1.38422900
C	8.23220800	-5.48118500	1.71852700
C	9.18527500	-5.53841700	2.72866600
C	9.85012300	-4.38654300	3.14036400
C	9.55642200	-3.17425800	2.52173200
C	8.61696000	-3.11213800	1.49932400
C	-0.53235800	1.79424100	2.21493600
C	0.41804500	0.87271100	2.65593900
C	1.10490400	1.07049500	3.84822000
C	0.85383700	2.19754000	4.62561600
C	-0.08345900	3.13068900	4.19338700
C	-0.76812600	2.92843000	2.99949800
C	0.56398400	1.64053600	-2.28110000
C	0.87088300	2.70921800	-3.13013800
C	0.19547100	2.88740300	-4.33299300
C	-0.80430600	1.99580500	-4.70917500
C	-1.12567700	0.93475200	-3.86761800
C	-0.44736000	0.76029100	-2.66683300
H	-4.35723900	1.35305800	-1.47447000
H	-2.21706700	3.63789800	-2.63269000
H	-3.91677400	3.59215700	-2.15627300

H	-3.38818800	4.93138900	-0.10794700
H	-2.89918700	5.79513900	-1.54648700
H	3.60446300	4.73254100	-0.08251100
H	3.12886200	5.68593200	1.31456300
H	4.02141900	3.46237600	2.03252400
H	2.31936100	3.62993900	2.47436000
H	4.34554000	1.17598700	1.45244200
H	-0.61516800	-1.61056900	1.22469800
H	-1.54329600	-2.30459800	2.58056800
H	-2.26996100	-2.22645400	0.95441400
H	0.45325100	-1.70105100	-1.13282600
H	1.35183400	-2.51584900	-2.44038500
H	2.06672700	-2.39612300	-0.81113200
H	-0.19593900	10.10375400	-2.13483800
H	-1.90188600	9.56565800	-2.00894400
H	-1.03046000	10.08873000	-0.54614800
H	4.24843100	8.67163700	-0.83487800
H	2.78018400	9.60054000	-0.38987900
H	3.71647200	8.77542800	0.87579000
H	-4.26520800	-1.11033400	-1.95737500
H	-5.98543900	-2.86527200	-1.93243400
H	-6.33999300	-2.44520400	2.31957300
H	-4.63085000	-0.67839500	2.28869000
H	4.09719000	-1.25900300	2.05496300
H	5.69618500	-3.12494500	2.13182600
H	6.16784500	-2.88580400	-2.12233100
H	4.54094700	-1.04323400	-2.20024400
H	-5.04761200	-5.20386000	-0.19156500
H	-4.80769100	-7.18689100	-1.64315300
H	-6.77013300	-8.07616700	-2.88212200
H	-8.97053800	-6.94286500	-2.65584400
H	-9.19910600	-4.94429600	-1.22476200
H	-8.38075200	-5.71606800	1.69343600
H	-10.37131800	-5.49559900	3.13708800
H	-11.53377800	-3.30820400	3.34121700
H	-10.68195700	-1.35118200	2.06786900
H	-8.70841200	-1.58310300	0.60377700
H	9.08798000	-5.27831100	-1.16913700
H	9.04651000	-7.04229500	-2.89546900
H	6.88109500	-7.97686900	-3.67943400
H	4.76080500	-7.12939900	-2.69824400

H	4.80864700	-5.38454500	-0.95181200
H	7.70952800	-6.37947400	1.40835900
H	9.39954800	-6.49018800	3.20471700
H	10.58882600	-4.43305900	3.93355900
H	10.07131300	-2.26860500	2.82690900
H	8.40005300	-2.16757100	1.01243400
H	0.63526500	-0.00218000	2.05447200
H	1.83945000	0.33923000	4.17146200
H	1.38488300	2.34712500	5.56049100
H	-0.29038500	4.01507100	4.78768800
H	-1.51020600	3.65235200	2.67807600
H	1.66092600	3.39920800	-2.85078600
H	0.45770300	3.71987500	-4.97838800
H	-1.32968000	2.12660400	-5.65003000
H	-1.90967800	0.23743700	-4.14650100
H	-0.72001100	-0.06177600	-2.01546200