Electronic Supplementary Information

P=O functional group-containing cryptands: from supramolecular complexes to poly[2]pseudorotaxanes

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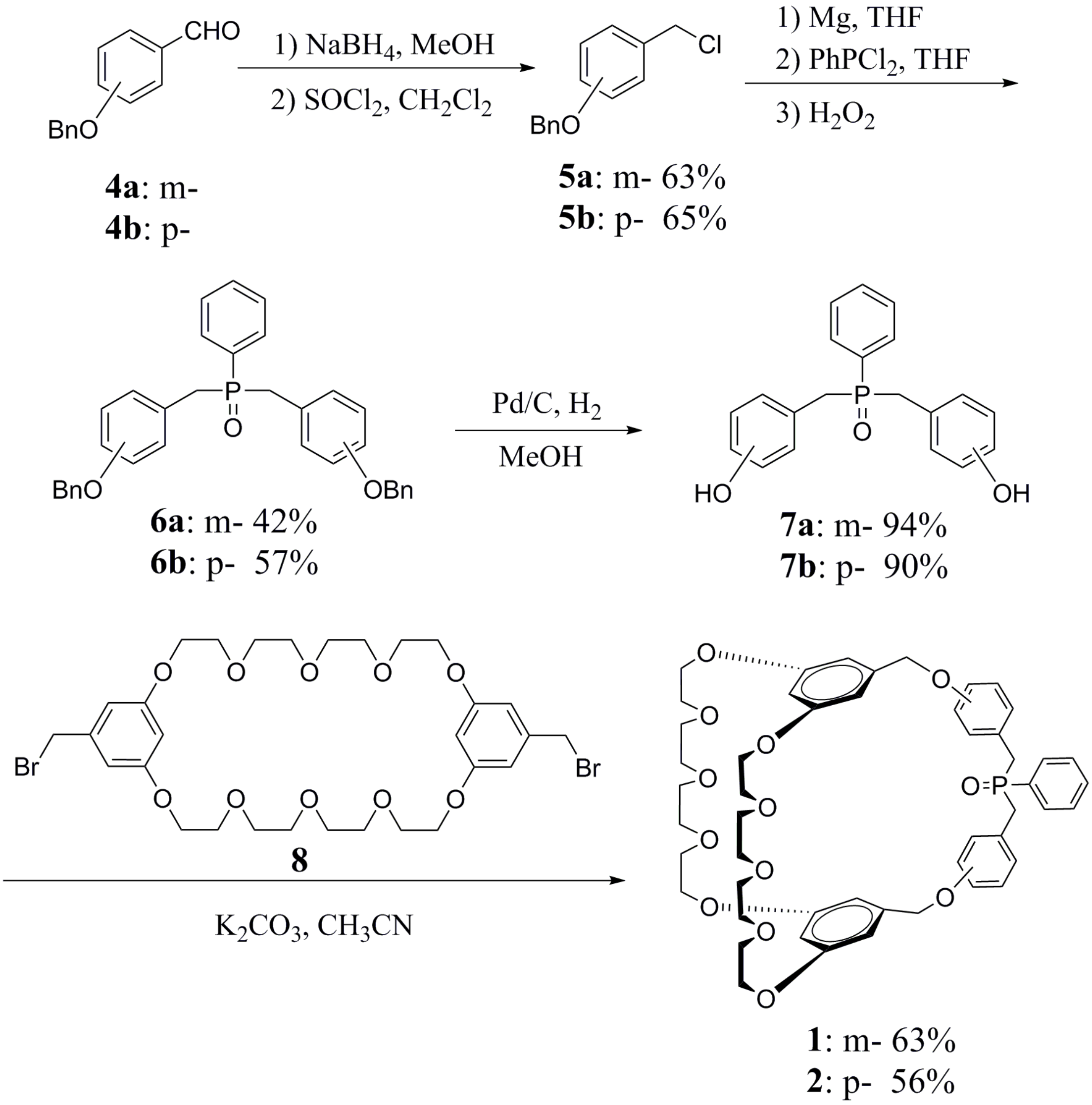
1. Materials and methods

All reactions were performed in atmosphere unless noted. The commercially available reagents and solvents were either employed as purchased or dried according to procedures described in the literature. Compounds 3,[S1] and 4[S2] were prepared according to literature procedure. NMR spectra were recorded on a Bruker DPX 300 MHz, 400 MHz or 500 MHz spectrometer with internal standard tetramethylsilane (TMS) and solvent signals as internal references, and the chemical shifts (δ) were expressed in ppm and *J* values were given in Hz. In the NMR spectra, the proton/carbon was not decoupled from phosphorus. 2D COSY and 2D NOESY experiments were performed on a Bruker DPX 400 MHz spectrometer. Low-resolution electrospray ionization mass spectra (LR-ESI-MS) were obtained on Finnigan MatTSQ 7000 instruments. High-resolution electrospray ionization mass spectra (HR-ESI-MS) were recorded on an Agilent 6540Q-TOF LCMS equipped with an electrospray ionization (ESI) probe operating in positive-ion mode with direct infusion.

2. *Synthesis of cryptands **1** and **2***



Scheme S1 Synthesis of cryptands **1** and **2**.

General procedure for the synthesis of 5: compound **4** (8.48 g, 39.95 mmol) was dissolved in methanol (120 mL), and then $NaBH_4$ (1.59 g, 42.03 mmol) was added. After 1 h, the solvent was removed by rotary evaporation. Then ethyl acetate (100 mL) and water (100 mL) were added. The organic layer was separated, and the aqueous phase was extracted with ethyl acetate (2 × 50 mL). The combined organic phases were then washed with water (50 mL) and brine (50 mL), and dried over anhydrous Na_2SO_4. The solvent was removed by rotary evaporation to give a white solid. The solid was dissolved in dry CH_2Cl_2 (50 mL), and then $SOCl_2$ (4.88 g, 41.02 mmol) was slowly added. After 20 h, the solvent was removed by rotary evaporation. The crude product was purified by column chromatography (silica, *n*-hexane/CH_2Cl_2 = 4/1, *v/v*).

5a[S3]: white solid. 5.86 g, 25.18 mmol, 63%.

5b[S3]: white solid. 6.04 g, 25.96 mmol, 65%.

General procedure for the synthesis of 6: A Schlenk flask was charged with magnesium powder (0.25 g, 10.28 mmol), anhydrous THF (20 mL), and 1,2-dibromoethane (0.10 mL, 1.15 mmol), Then compound **5** (2.05 g, 8.81 mmol) in anhydrous THF (5 mL) was added dropwise with stirring. After 3 h, a solution of $PhPCl_2$ (0.72 g, 4.02 mmol) in anhydrous THF (5 mL) was added. After 20 h, saturated aqueous NH_4Cl (4 mL) was added. The mixture was filtered and the filtrate was removed by rotary evaporation. Subsequently, CH_2Cl_2 (50 mL) and H_2O_2 (1 mL) was added and stirred for about half an hour. The mixture was dried over anhydrous Na_2SO_4. The solvent was removed by rotary evaporation. The crude product was purified by column chromatography (silica, CH_2Cl_2/AcOEt = 10/1, *v/v*).

6a: white solid, 0.88 g, 1.70 mmol, 42%. M.p. 142−143 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) δ (ppm): 7.56−7.28 (m, 15H), 7.14 (t, J = 7.9 Hz, 2H), 6.82 (d, J = 8.2 Hz, 2H), 6.74−6.71 (m, 4H), 4.94 (s, 4H), 3.31 (d, J = 13.9 Hz, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K) δ (ppm): 158.9, 137.0, 133.0 (d, J = 7.4 Hz), 131.9, 131.3 (d, J = 8.5 Hz), 129.7, 128.7, 128.4 (d, J = 11.4 Hz), 128.1, 127.6, 122.8 (d, J = 5.0 Hz), 116.3 (d, J = 4.8 Hz), 114.0, 69.9, 37.6 (d, J = 63.2 Hz). ^{31}P NMR (500 MHz, $CDCl_3$, 298 K) δ (ppm): 34.8 (s). LR-ESI-MS: *m*/*z* calcd. for $[M + H]^+$ = 519.21, found 519.15 (100%); $[M + Na]^+$ = 541.19, found 541.15 (80%). HR-ESI-MS: *m*/*z* calcd. for $[M + H]^+$ $C_{34}H_{32}O_3P^+$, 519.2089, found 519.2087, error −0.4 ppm.

6b: white solid, 1.19 g, 2.29 mmol, 57%. M.p. 188−190 °C. ^{1}H NMR (300 MHz, $CDCl_3$, 298 K) δ (ppm): 7.54−7.31 (m, 15H), 7.03 (dd, J_1 = 8.6 Hz, J_2 = 1.9 Hz, 4H), 6.84 (d, J = 8.6 Hz, 4H), 5.01 (s, 4H), 3.27 (d, J = 13.5 Hz, 4H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K) δ (ppm): 157.9, 137.1, 131.8, 131.3 (d, J = 8.8 Hz), 131.1 (d, J = 5.0 Hz), 128.7, 128.4 (d, J = 11.3 Hz), 128.1, 127.6, 123.7 (d, J = 7.5 Hz), 115.1, 70.1, 36.5 (d, J = 64.0 Hz). ^{31}P NMR (500 MHz, $CDCl_3$, 298 K) δ (ppm): 35.2 (s). LR-ESI-MS: m/z calcd. for $[M + H]^+$ = 519.21, found: 519.15 (100%); $[M + Na]^+$ = 541.19, found 541.15 (33%). HR-ESI-MS: m/z calcd for $[M + H]^+$ $C_{34}H_{32}O_3P^+$, 519.2089, found 519.2088, error −0.2 ppm.

General procedure for the synthesis of 7: A Schlenk flask was charged with **6** (1.60 g, 3.09 mmol) and 10% Pd/C (0.30 g) in MeOH (30 mL), and the above mixture was stirred at 25 °C under H_2 for 24 h. The mixture was filtered and the filtrate was removed by rotary evaporation to give **7** as a white solid.

7a: 0.99 g, 2.93 mmol, 94%. M.p. 107−108 °C. ^{1}H NMR (300 MHz, DMSO-d_6, 298 K) δ (ppm): 9.24 (s, 2H), 7.70−7.64 (m, 2H), 7.51−7.37 (m, 3H), 6.94 (t, J = 7.7 Hz, 2H), 6.54−6.51 (m, 4H), 6.46 (d, J = 7.4 Hz, 2H), 3.37−3.30 (m, 4H). ^{13}C NMR (75 MHz, DMSO-d_6, 298 K) δ (ppm): 157.0, 133.7 (d, J = 7.9 Hz), 132.6, 131.3, 131.1 (d, J = 8.9 Hz), 128.9, 128.1 (d, J = 11.1 Hz), 120.6 (d, J = 4.8 Hz), 116.9 (d, J = 4.6 Hz), 113.3, 36.8 (d, J = 62.7 Hz). ^{31}P NMR (500 MHz, DMSO-d_6, 298 K) δ (ppm): 35.1 (s). LR-ESI-MS: m/z calcd. for $[M + H]^+$ = 339.12, found: 339.05 (100%); $[M + Na]^+$ = 361.10, found 361.05 (31%). HR-ESI-MS: m/z calcd. for $[M + H]^+$ $C_{20}H_{20}O_3P^+$, 339.1150, found 339.1161, error 3.2 ppm.

7b: 0.95 g, 2.81 mmol, 90%. M.p. 214−216 °C. ^{1}H NMR (300 MHz, DMSO-d_6, 298 K) δ (ppm): 9.17 (s, 2H), 7.64−7.58 (m, 2H), 7.48−7.39 (m, 3H), 6.85 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 4H), 6.55 (d, J = 8.4 Hz, 4H), 3.30−3.18 (m, 4H). ^{13}C NMR (75 MHz, DMSO-d_6, 298 K) δ (ppm): 155.8, 132.8, 131.6, 131.2, 131.1 (d, J = 8.7 Hz), 130.7 (d, J = 4.8 Hz), 128.1 (d, J = 10.9 Hz), 122.3 (d, J = 8.2 Hz), 115.0, 35.6 (d, J = 63.6 Hz). ^{31}P NMR (500 MHz, DMSO-d_6, 298 K) δ (ppm): 34.5 (s). LR-ESI-MS: m/z calcd. for $[M + H]^+$ = 339.12, found 339.05 (100%); $[M + Na]^+$ = 361.10, found 361.05 (20%). HR-ESI-MS: m/z calcd. for $[M + H]^+$ $C_{20}H_{20}O_3P^+$, 339.1150, found 339.1151, error 0.3 ppm.

General procedure for the synthesis of 1 and 2: A mixture of **7** (0.10 g, 0.30 mmol) and **8** (0.22 g, 0.30 mmol) in anhydrous CH_3CN (60 mL) was added very slowly to a suspension containing K_2CO_3 (0.25 g, 1.81 mmol) in anhydrous CH_3CN (150 mL) at reflux temperature under nitrogen gas protection. After complete addition, the mixture was stirred at reflux temperature for 2 days. After the solvent was removed by rotary evaporation, the residue was purified by column chromatography (silica, CH_2Cl_2/CH_3OH = 100/1, *v/v*).

1: white solid, 0.17 g, 0.19 mmol, 63%, M.p. 48−50 °C. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ (ppm): 7.51−7.38 (m, 5H), 7.09 (t, J = 7.9 Hz, 2H), 6.82 (d, J = 8.2 Hz, 2H), 6.65 (d, J = 7.5 Hz, 2H), 6.59 (s, 2H), 6.47 (d, J = 1.8 Hz, 4H), 6.30 (t, J = 1.9 Hz, 2H), 4.92−4.85 (m, 4H), 3.92−3.89 (m, 8H), 3.78−3.76 (m, 8H), 3.68−3.65 (m, 16H), 3.30−3.14 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ (ppm): 160.2, 158.5 (d, J = 2.2 Hz), 139.1, 132.6 (d, J = 7.3 Hz), 132.2, 131.1 (d, J = 8.6 Hz), 129.7, 128.5 (d, J = 11.5 Hz), 122.9 (d, J = 5.2 Hz), 116.0 (d, J = 5.7 Hz), 114.5, 106.0, 100.9, 71.0, 70.8, 69.8, 69.7, 67.6, 37.0 (d, J = 62.9 Hz). ^{31}P NMR (400 MHz, $CDCl_3$, 298 K) δ (ppm): 48.4 (s). LR-ESI-MS: *m*/*z* calcd. for $[M + H]^+$ = 899.38, found 899.40 (100%); $[M + NH_4]^+$ = 916.40, found 916.40 (75%); $[M + Na]^+$ = 921.36, found 921.35 (58%); $[M + K]^+$ = 937.33, found 937.30 (31%). HR-ESI-MS: *m*/*z* calcd. for $[M + Na]^+$ $C_{50}H_{59}NaO_{13}P^+$, 921.3591, found 921.3591, error 0.0 ppm.

2: white solid, 0.15 g, 0.17 mmol, 56%, M.p. 63−65 °C. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) δ (ppm): 7.61−7.41 (m, 5H), 6.90 (dd, J_1 = 8.4 Hz, J_2 = 1.5 Hz, 4H), 6.64 (d, J = 8.5 Hz, 4H), 6.44 (d, J = 2.0 Hz, 4H), 6.33 (t, J = 2.0 Hz, 4H), 4.95 (s, 4H), 3.98−3.95 (m, 8H), 3.80−3.78 (m, 8H), 3.67−3.66 (m, 16H), 3.31−3.11 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) δ (ppm): 160.2, 157.3 (d, J = 2.7 Hz), 139.6, 132.1 (d, J = 2.1 Hz), 131.0 (d, J = 5.5 Hz), 130.9, 128.6 (d, J = 11.3 Hz), 123.3 (d, J = 7.4 Hz), 115.3 (d, J = 1.9 Hz), 105.5, 100.7, 70.92, 70.85, 69.8, 67.6, 36.3 (d, J = 64.2 Hz). ^{31}P NMR (400 MHz, $CDCl_3$, 298 K) δ (ppm): 35.9 (s). LR-ESI-MS: *m*/*z* calcd. for $[M + H]^+$ = 899.38, found 899.55 (20%); $[M + NH_4]^+$ = 916.40, found 916.55 (40%); $[M + K]^+$ = 937.33, found 937.50 (100%). HR-ESI-MS: *m*/*z* calcd. for $[M + Na]^+$ $C_{50}H_{59}NaO_{13}P^+$, 921.3591, found 921.3587, error −0.4 ppm.

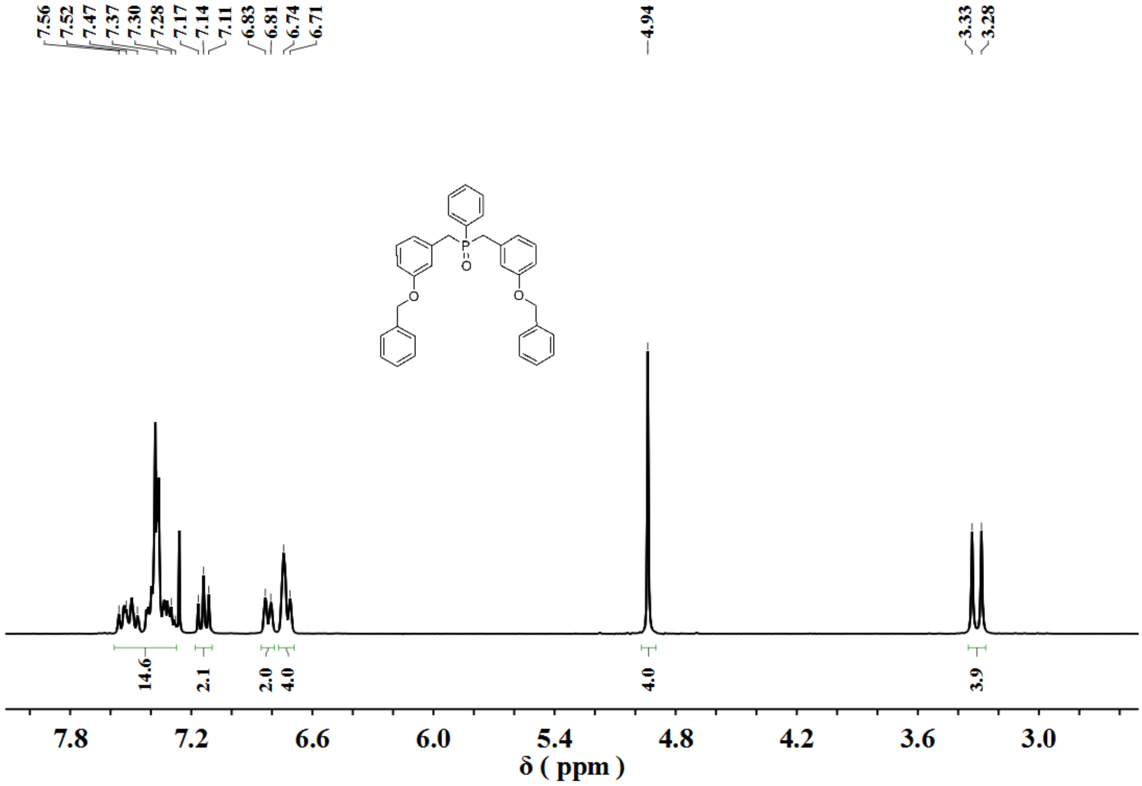


Fig. S1 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of **6a**.

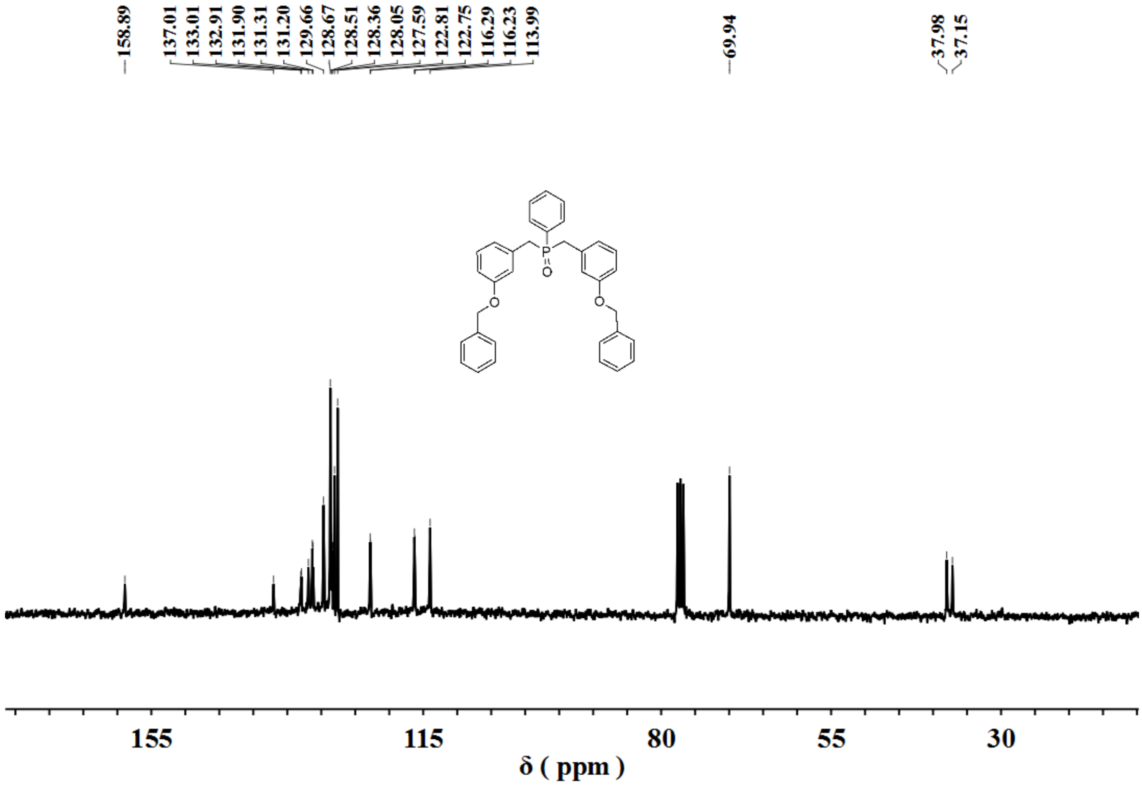


Fig. S2 ^{13}C NMR spectrum (75 MHz, $CDCl_3$, 298 K) of **6a**.

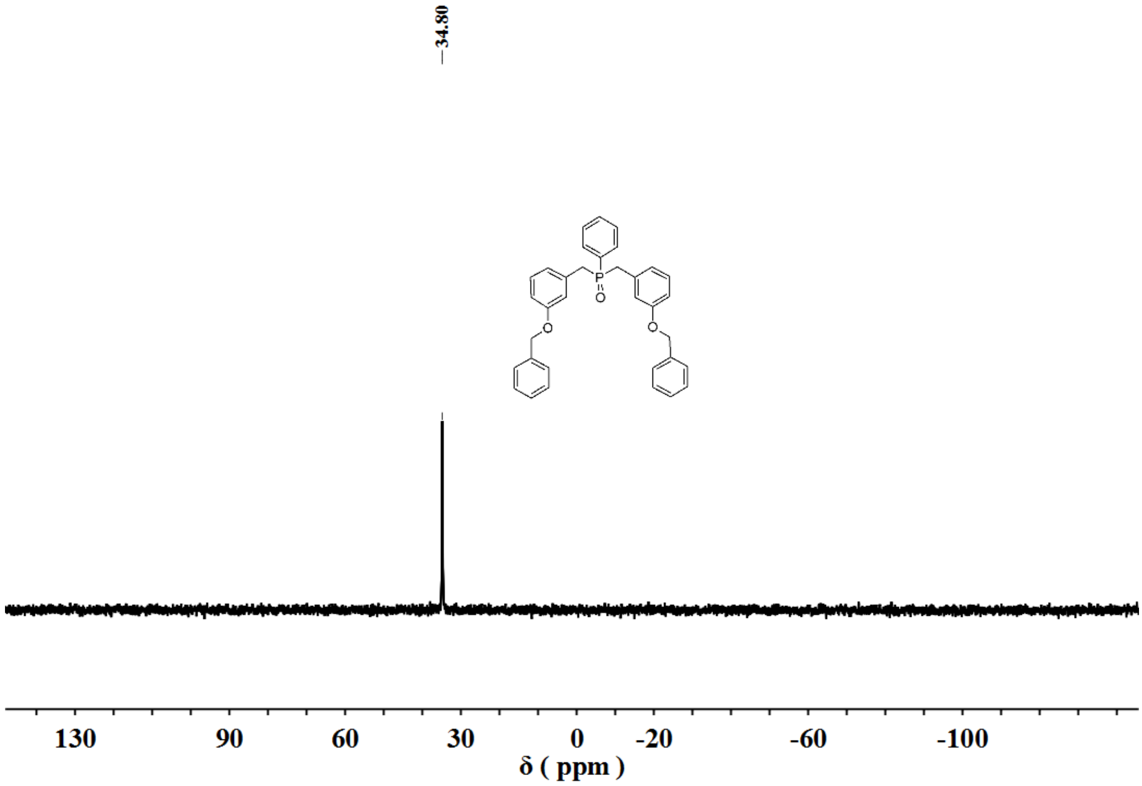


Fig. S3 ^{31}P NMR spectrum (500 MHz, $CDCl_3$, 298 K) of **6a**.

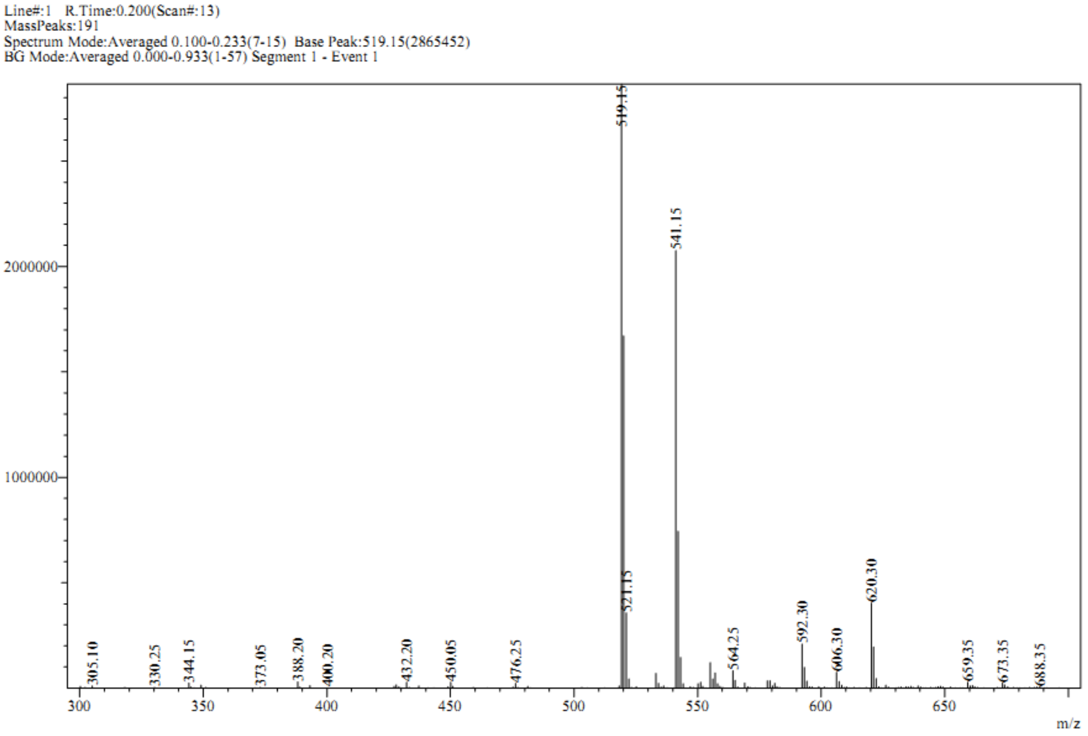


Fig. S4 LR-ESI-MS spectrum of **6a**.

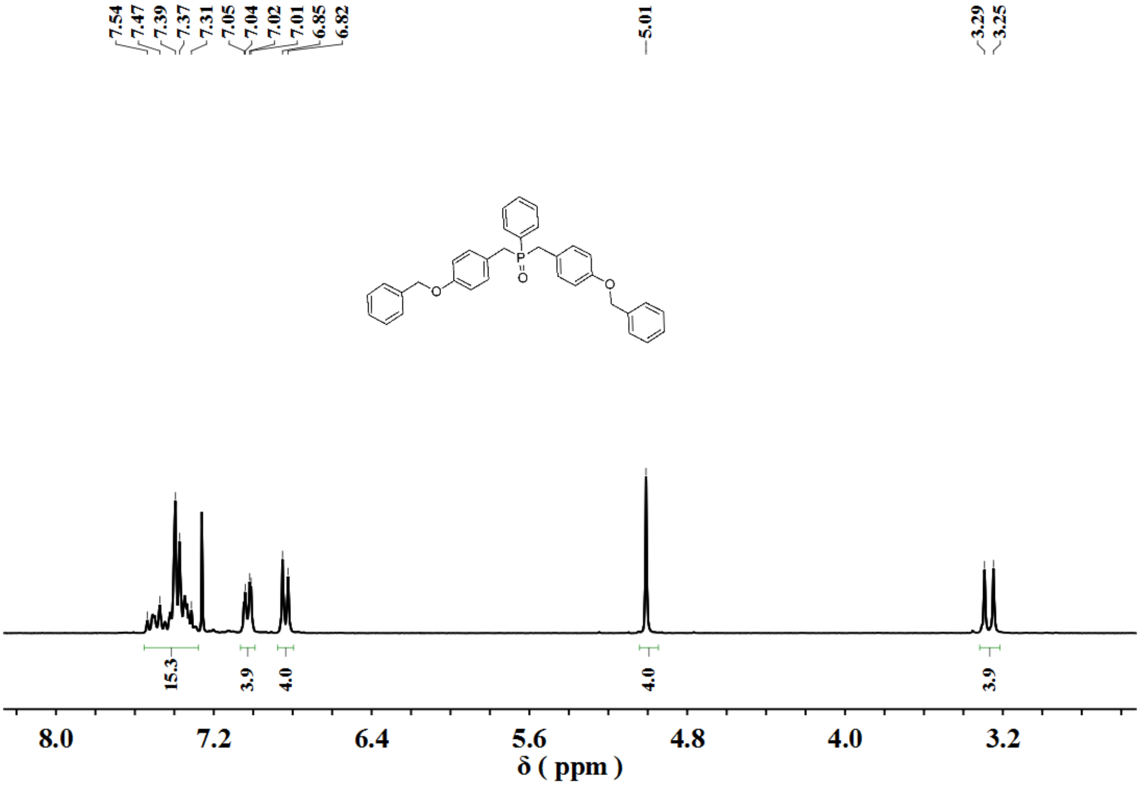


Fig. S5 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of **6b**.

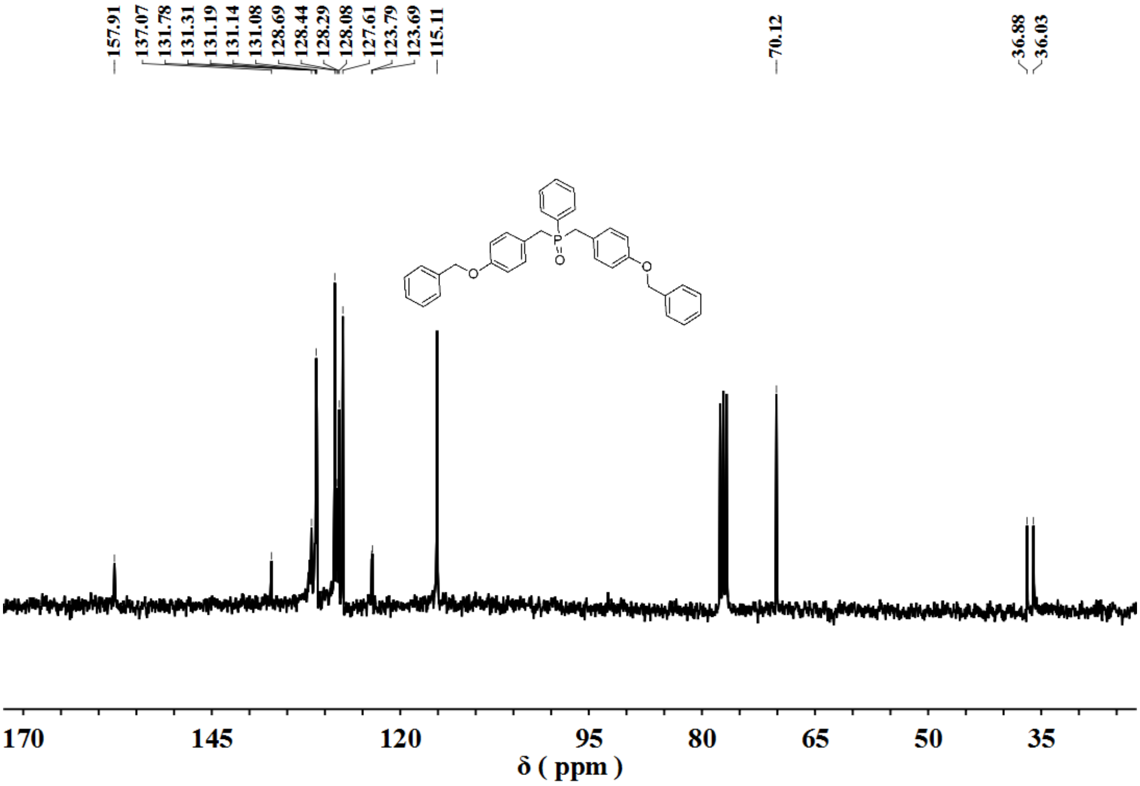


Fig. S6 ^{13}C NMR spectrum (75 MHz, $CDCl_3$, 298 K) of **6b**.

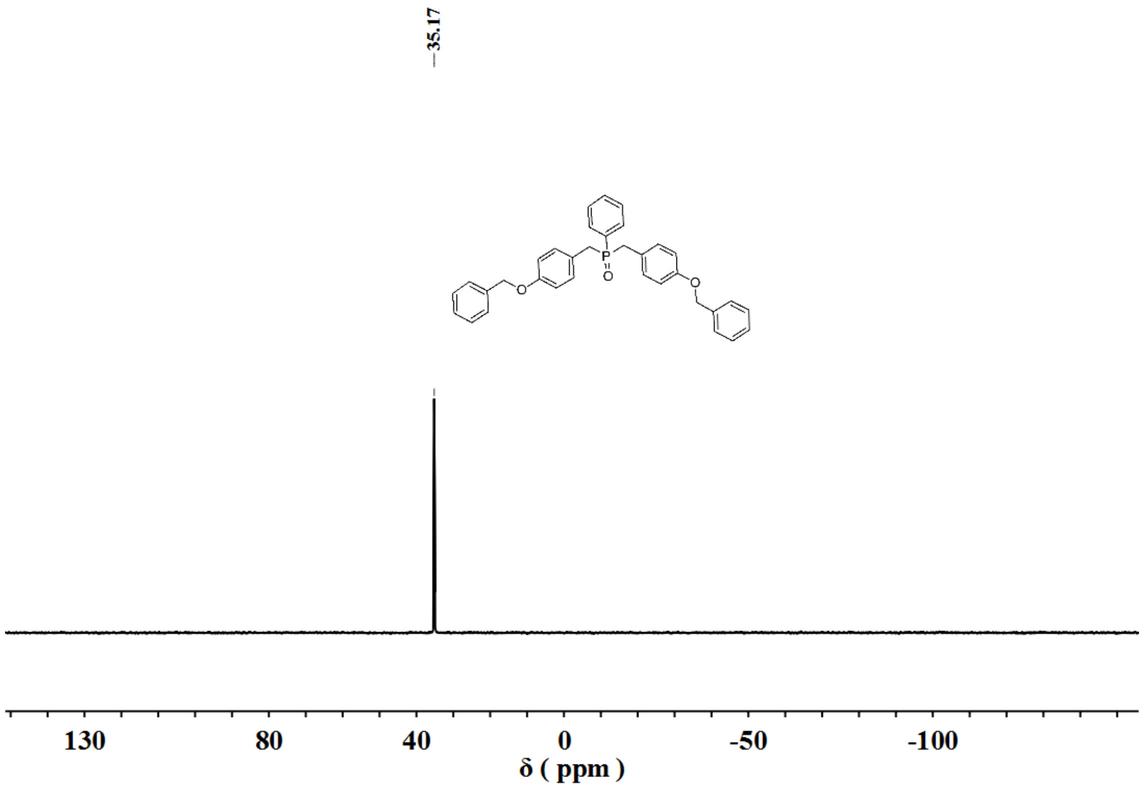


Fig S7 ^{31}P NMR spectrum (500 MHz, CDCl$_3$, 298 K) of **6b**.

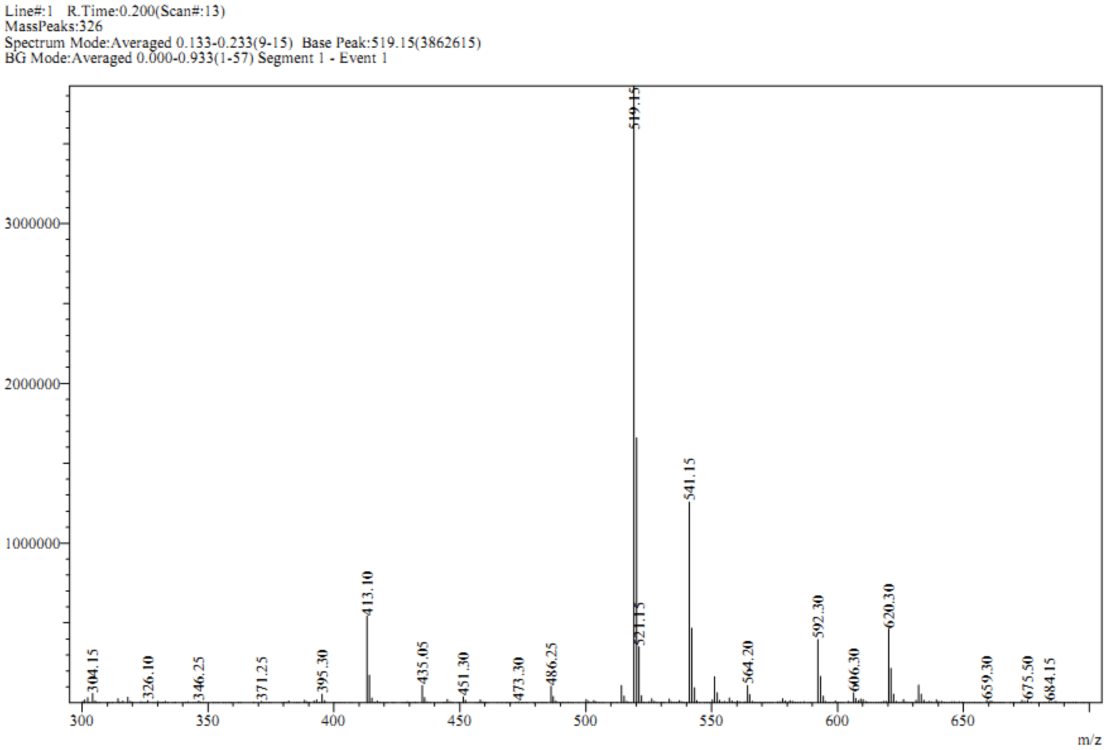


Fig. S8 LR-ESI-MS spectrum of **6b**.

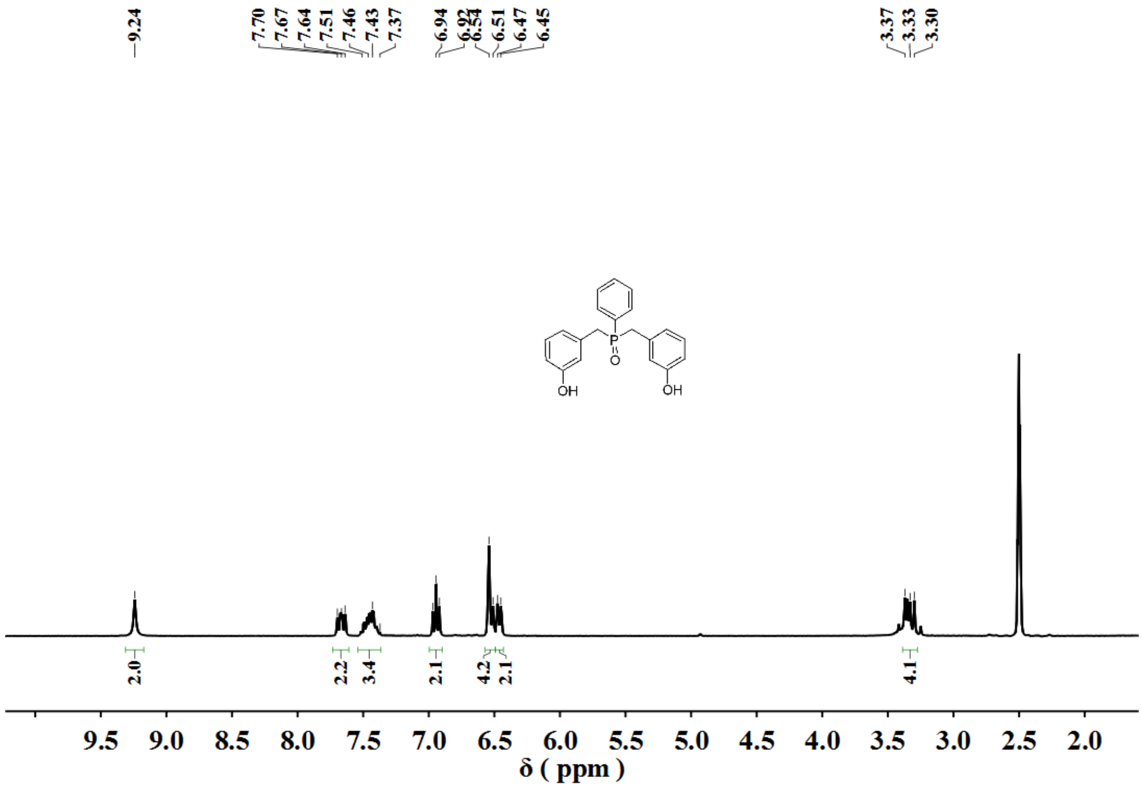


Fig. S9 ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 298 K) of **7a**.

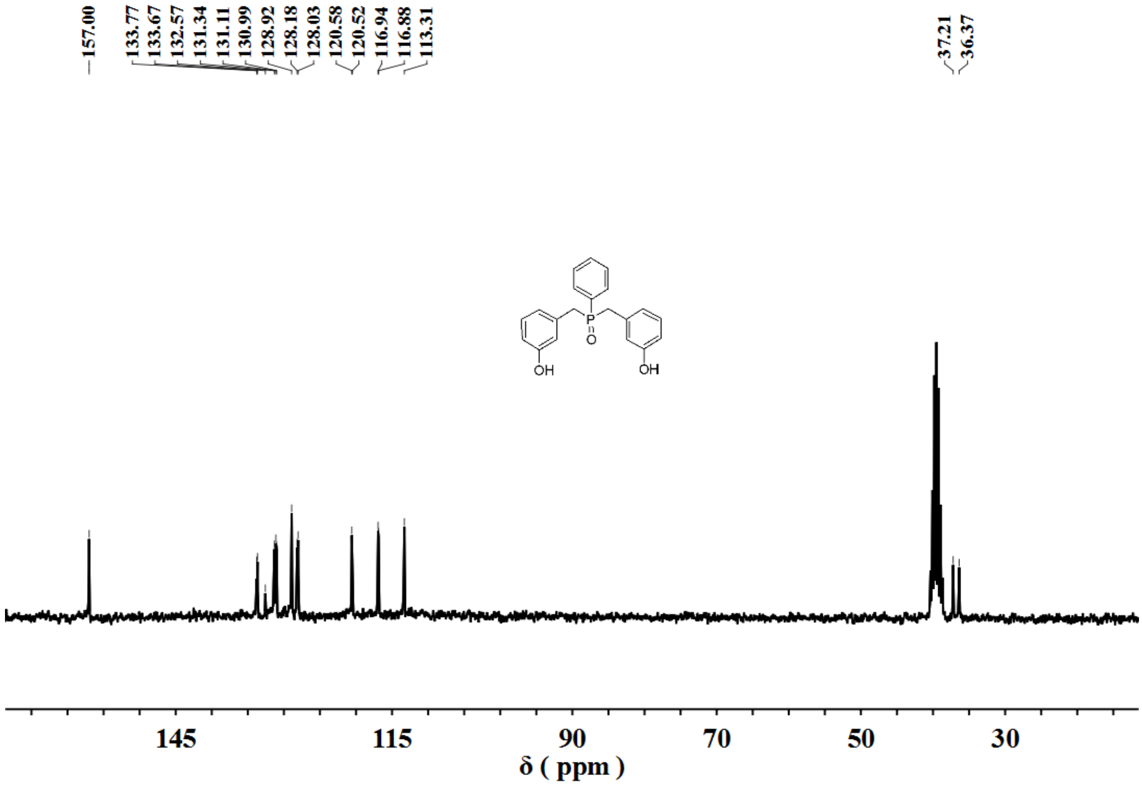


Fig. S10 ^{13}C NMR spectrum (75 MHz, DMSO-d_6, 298 K) of **7a**.

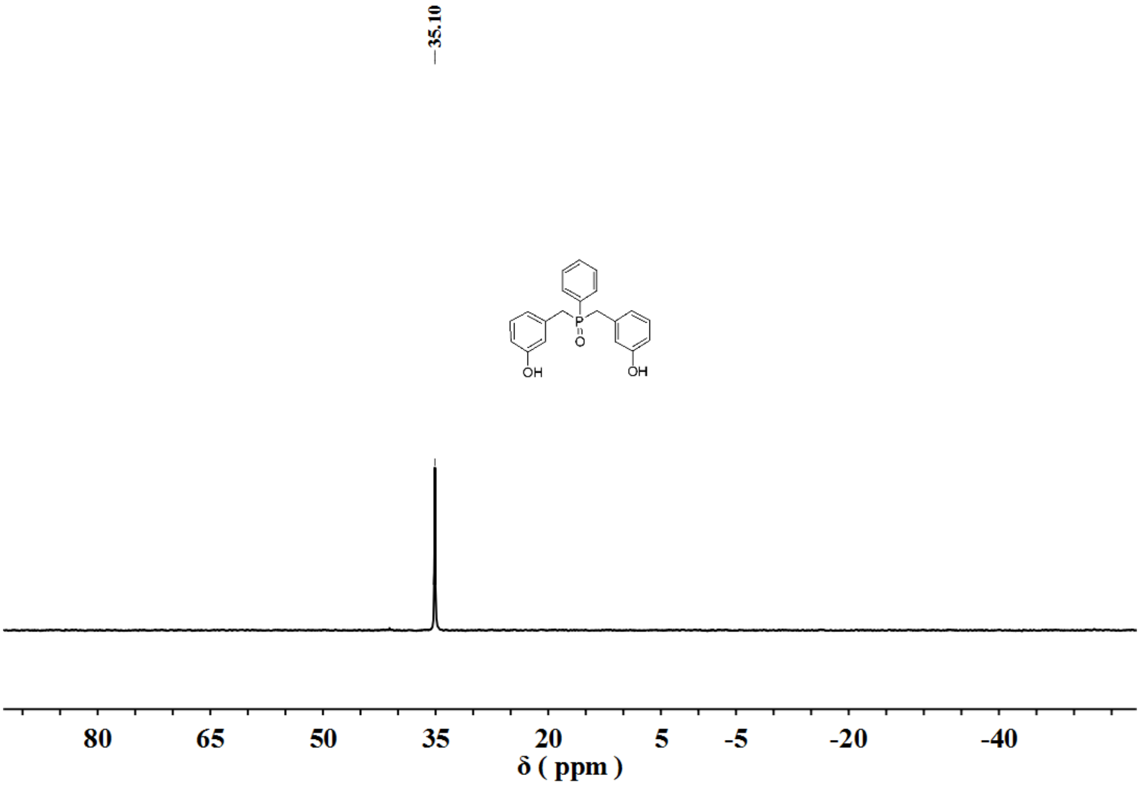


Fig. S11 ^{31}P NMR spectrum (500 MHz, DMSO-d_6, 298 K) of **7a**.

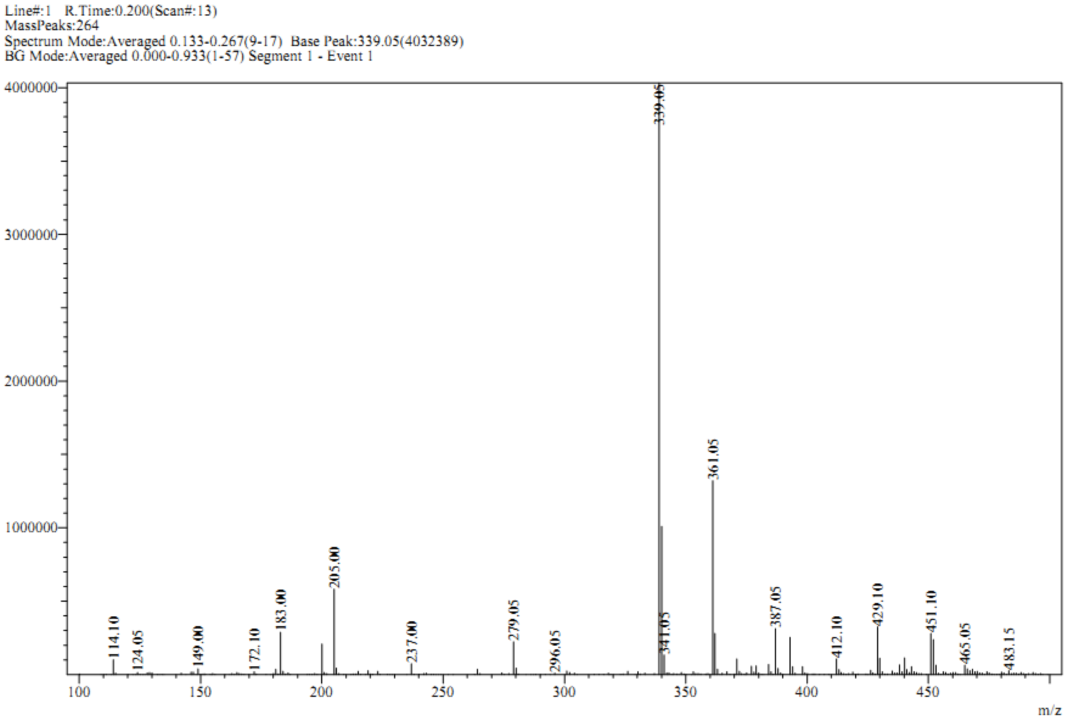


Fig. S12 LR-ESI-MS spectrum of **7a**.

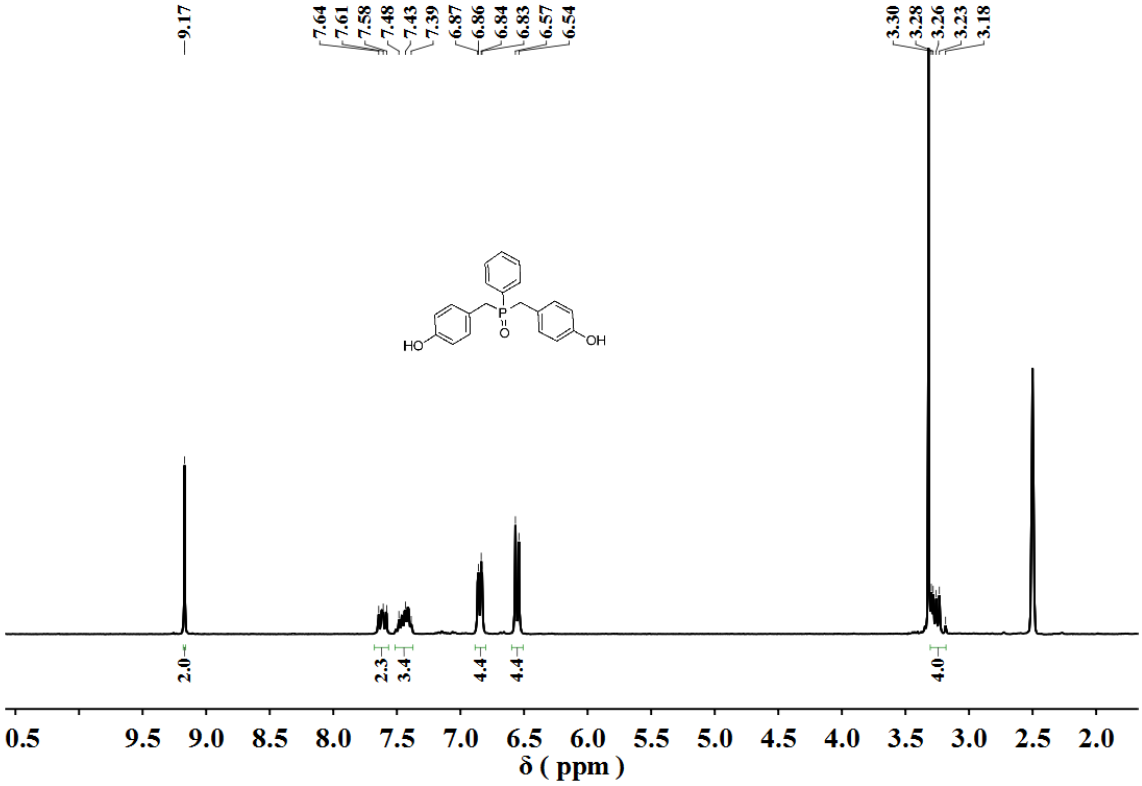


Fig. S13 ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 298 K) of **7b**.

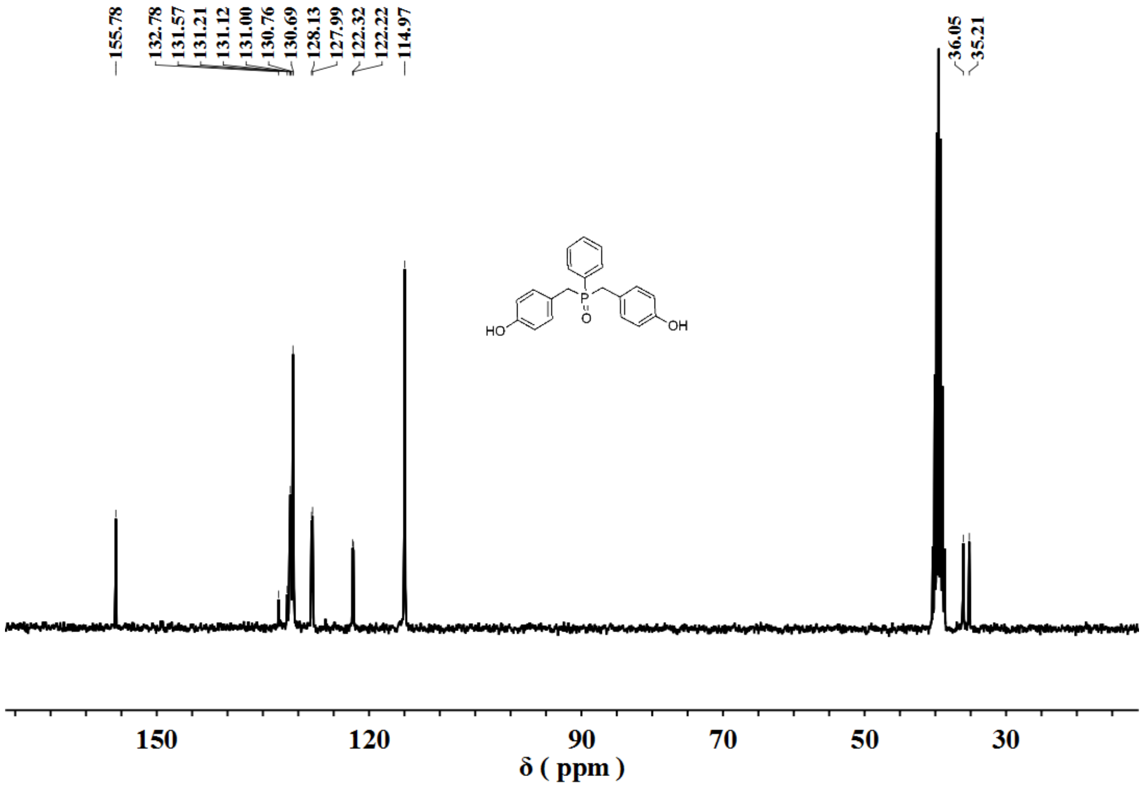


Fig. S14 ^{13}C NMR spectrum (75 MHz, DMSO-d_6, 298 K) of **7b**.

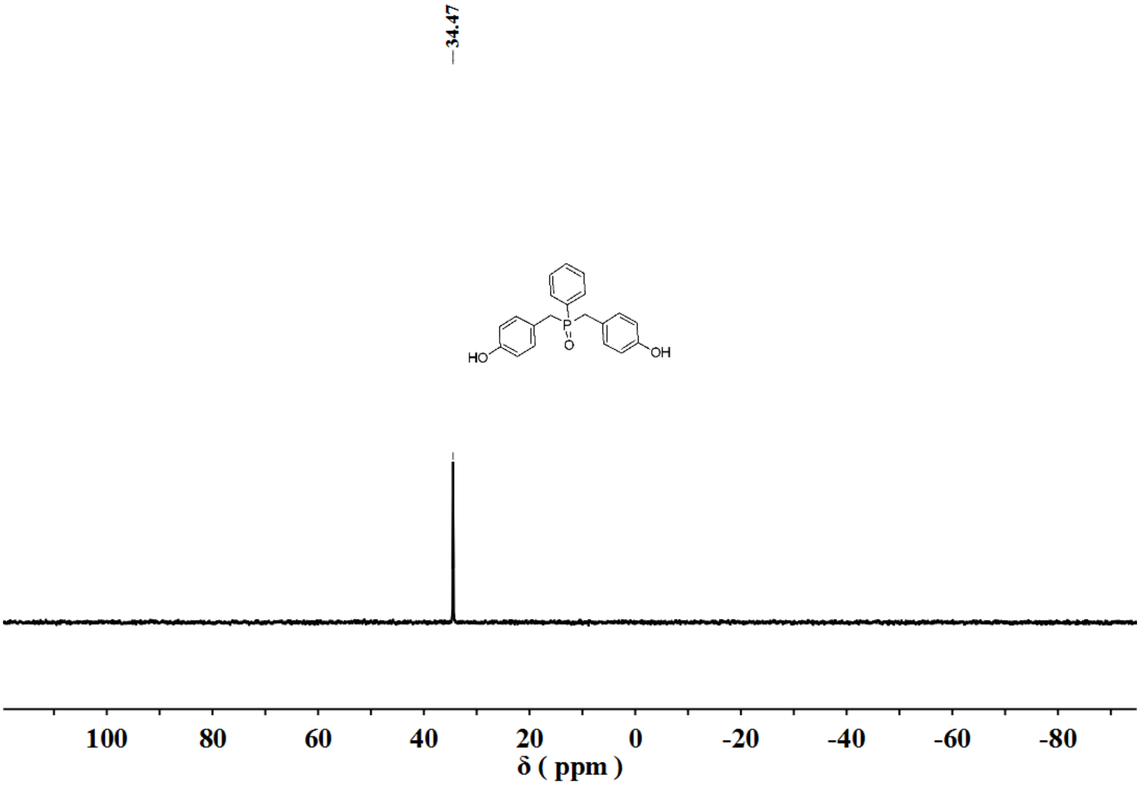


Fig. S15 ^{31}P NMR spectrum (500 MHz, DMSO-d_6, 298 K) of **7b**.

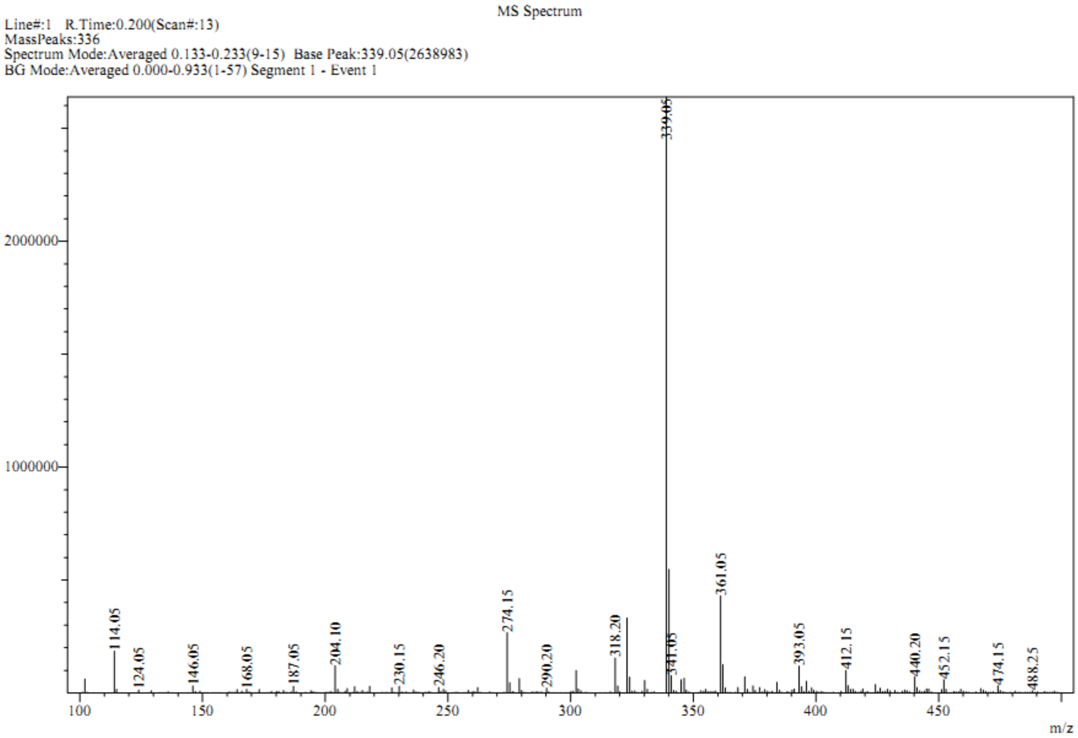


Fig. S16 LR-ESI-MS spectrum of **7b**.

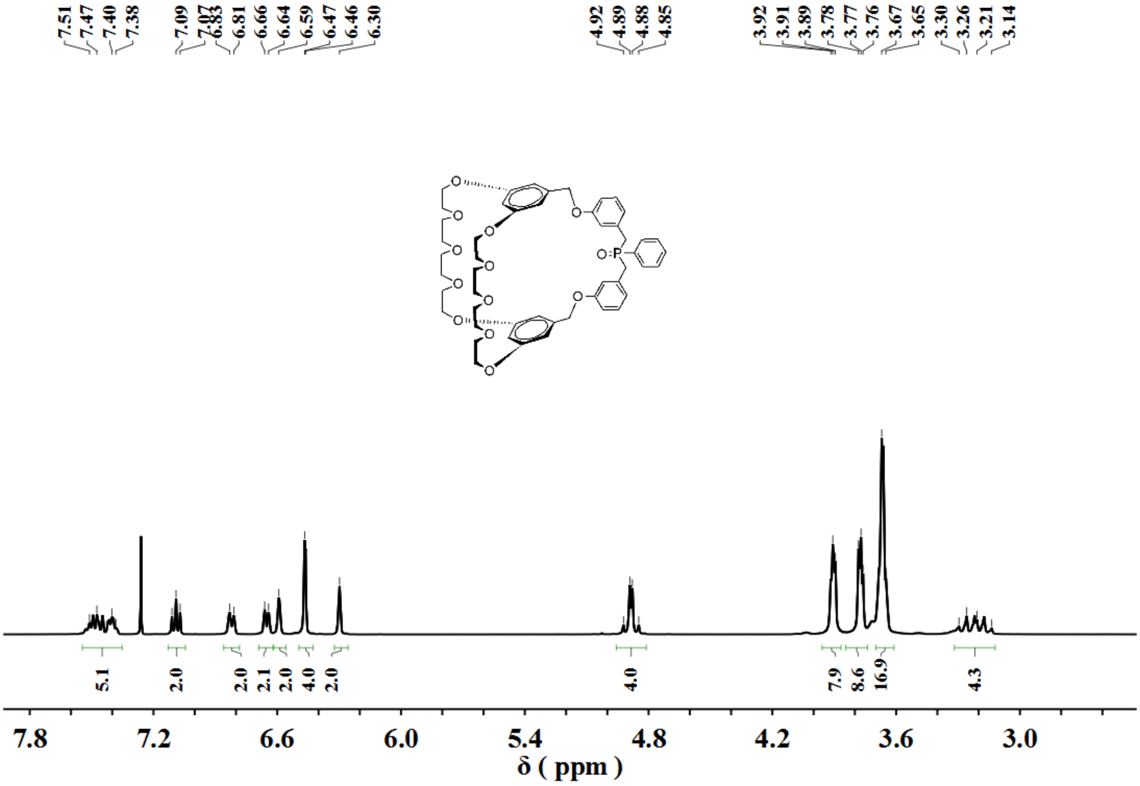


Fig. S17 ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **1**.

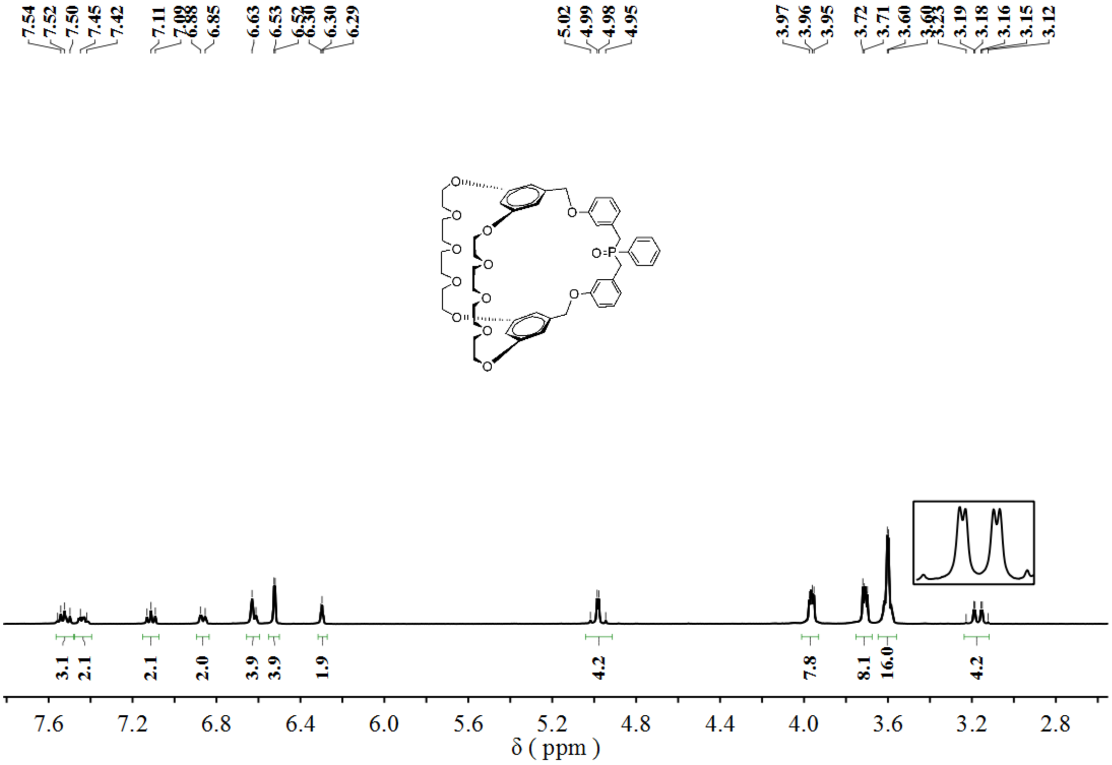


Fig. S18 ^{1}H NMR spectrum (400 MHz, CD_3CN, 298 K) of **1**.

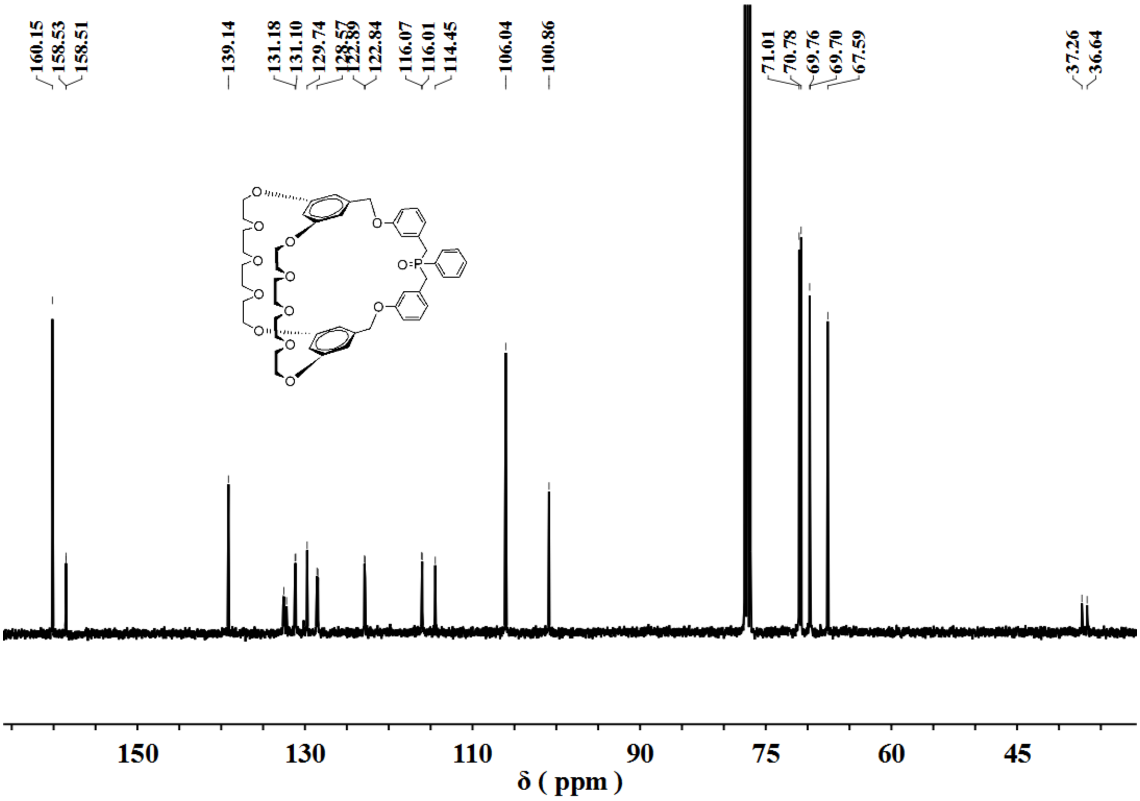


Fig. S19 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **1**.

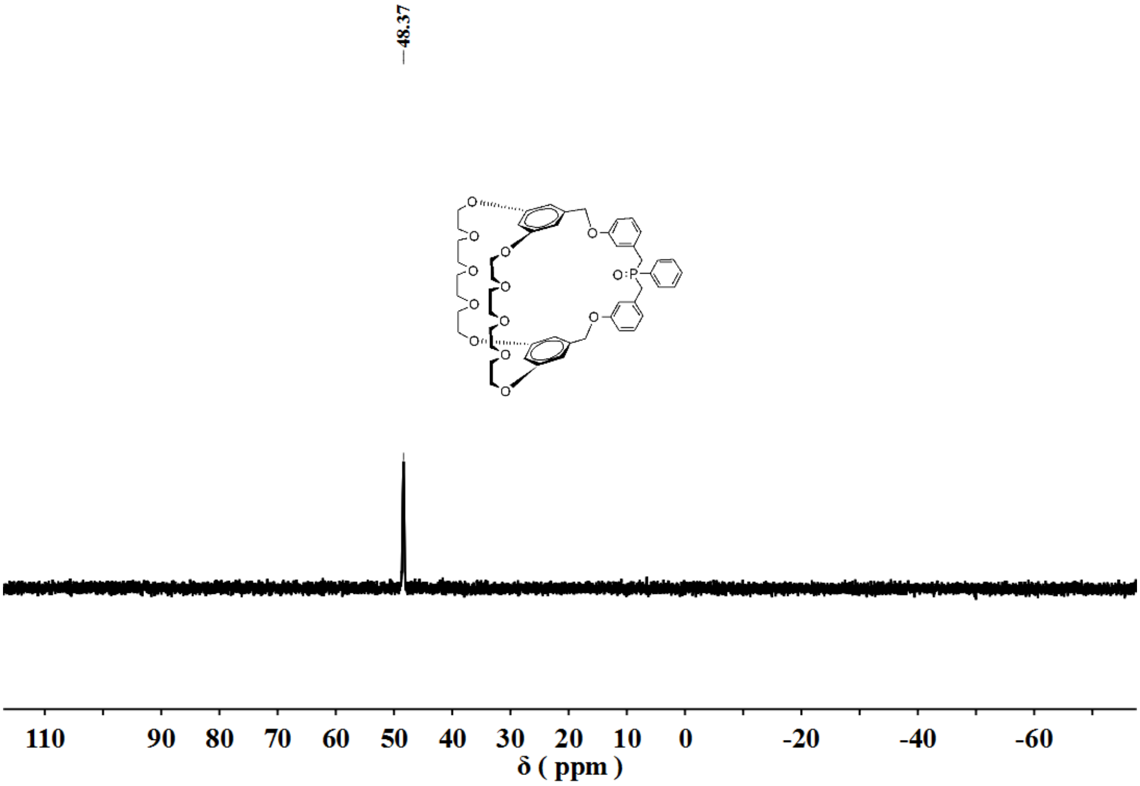


Fig. S20 ^{31}P NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **1**.

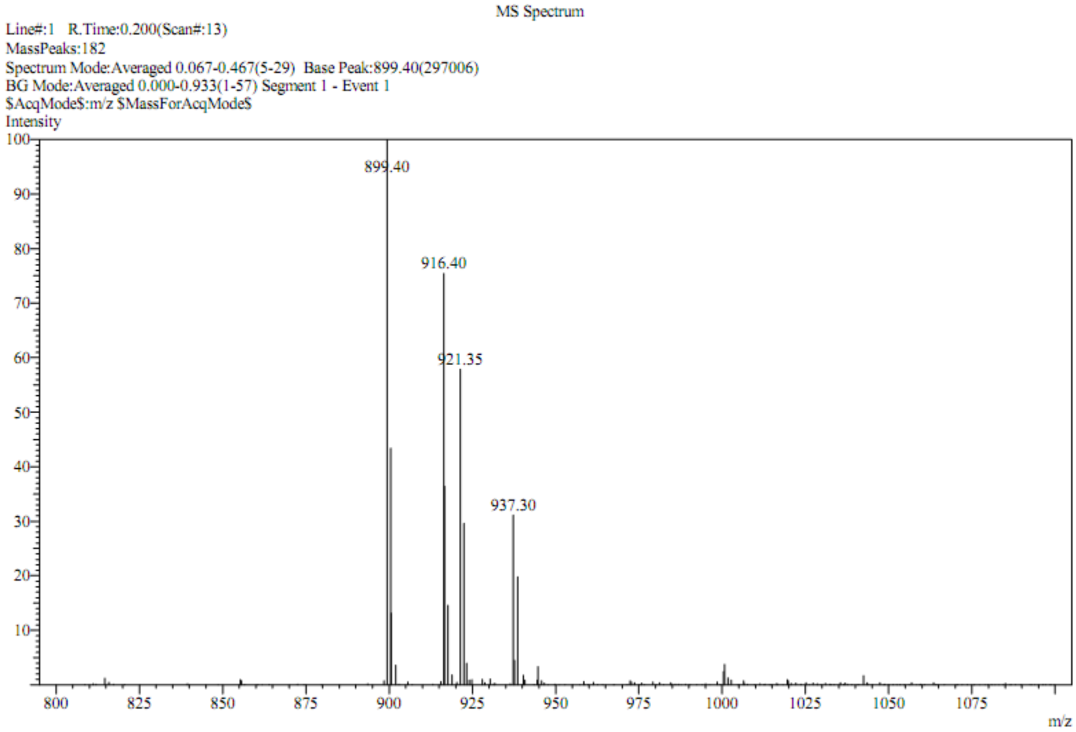


Fig. S21 LR-ESI-MS spectrum of **1**.

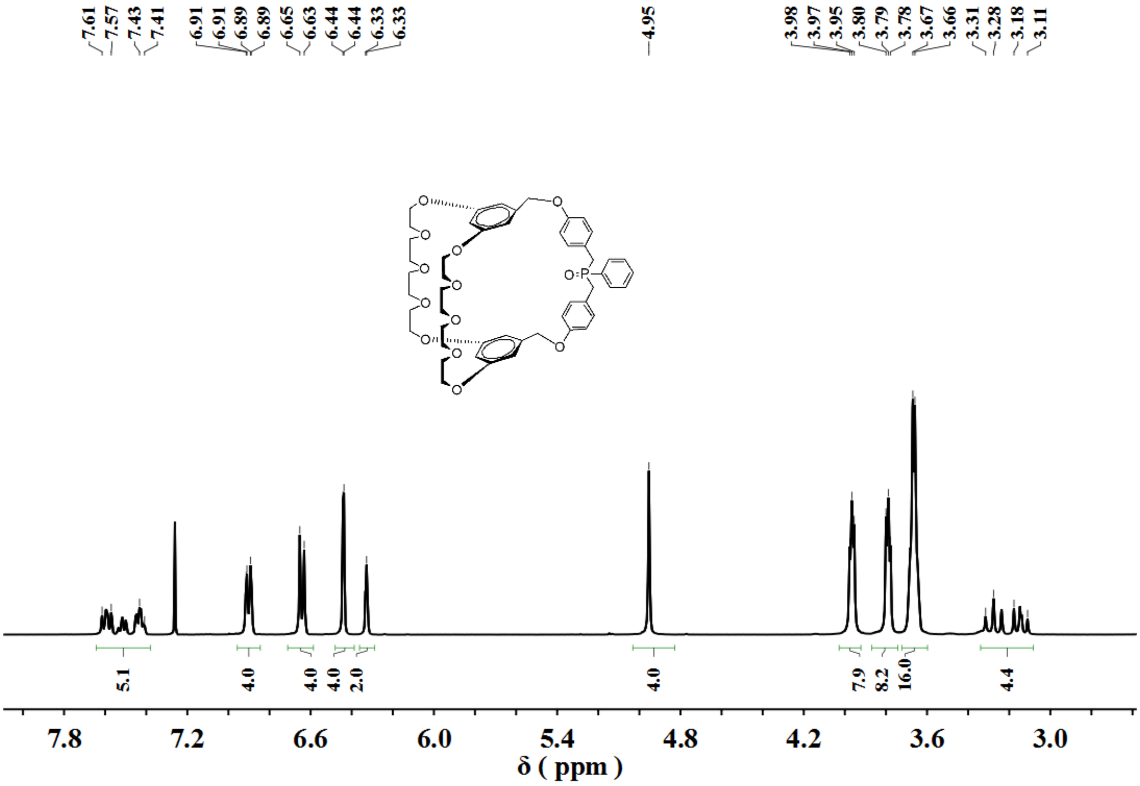


Fig. S22 ^{1}H NMR spectrum (400 MHz, CDCl$_3$, 298 K) of **2**.

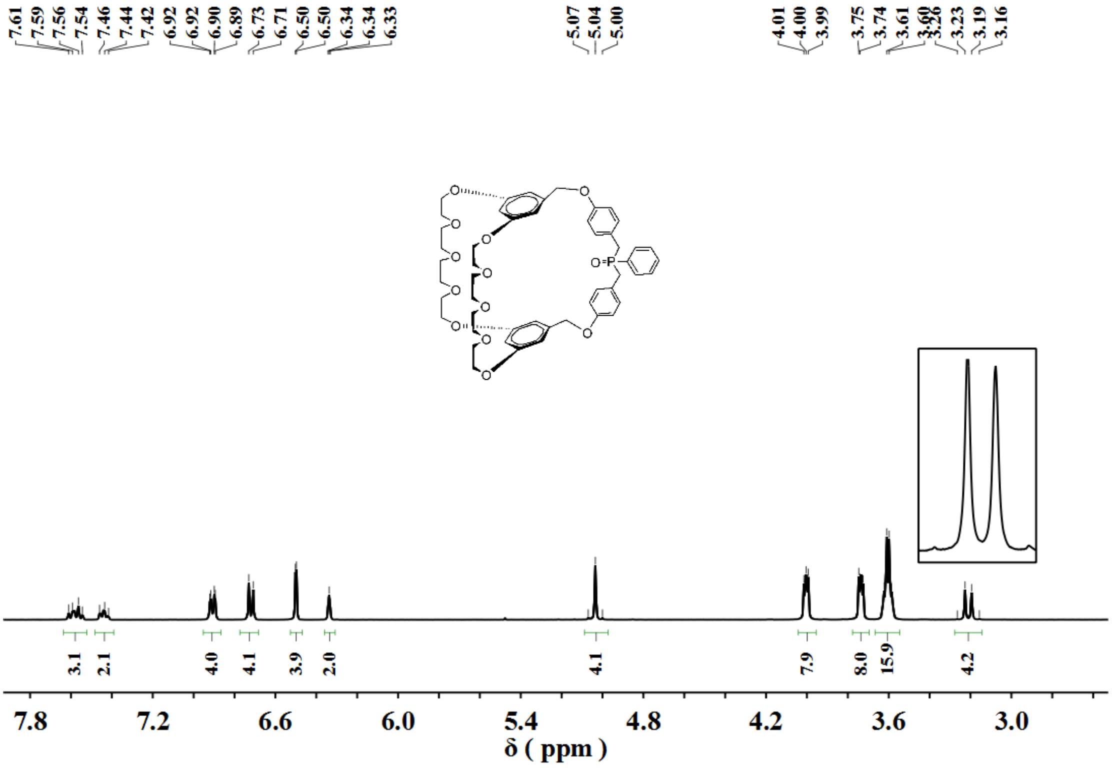


Fig. S23 ^{1}H NMR spectrum (400 MHz, CD_3CN, 298 K) of **2**.

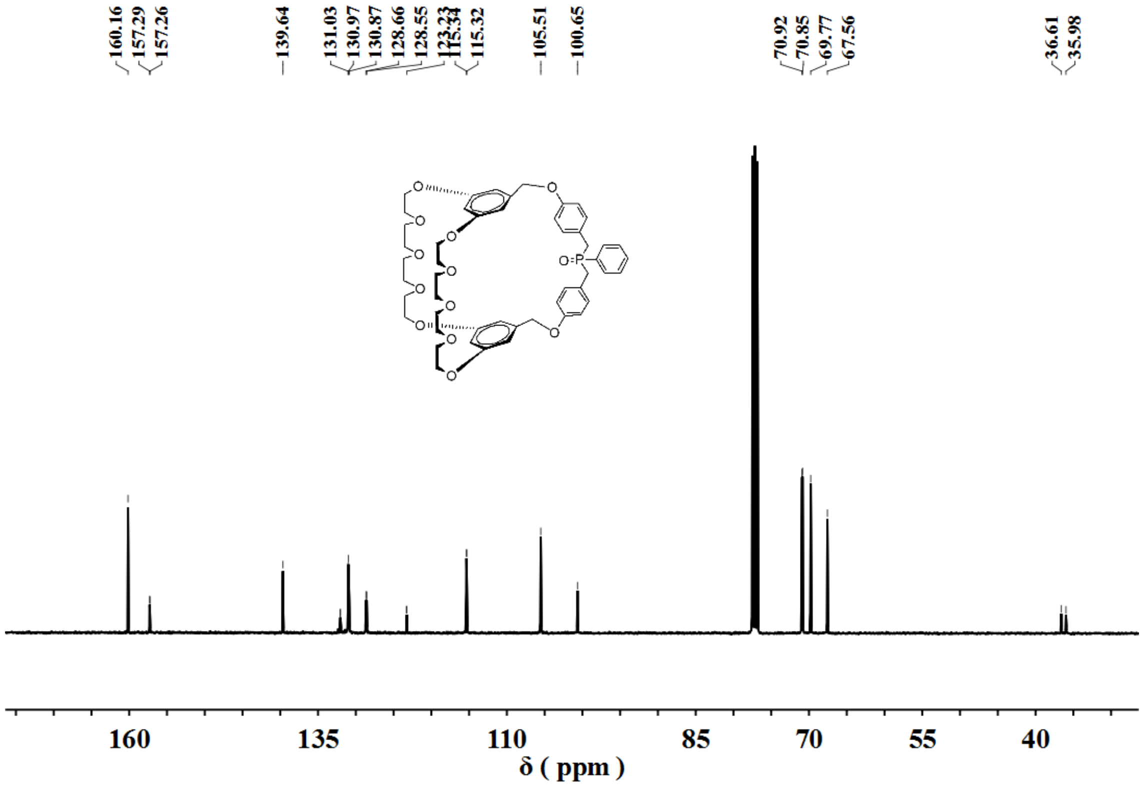


Fig. S24 ^{13}C NMR spectrum (100 MHz, $CDCl_3$, 298 K) of **2**.

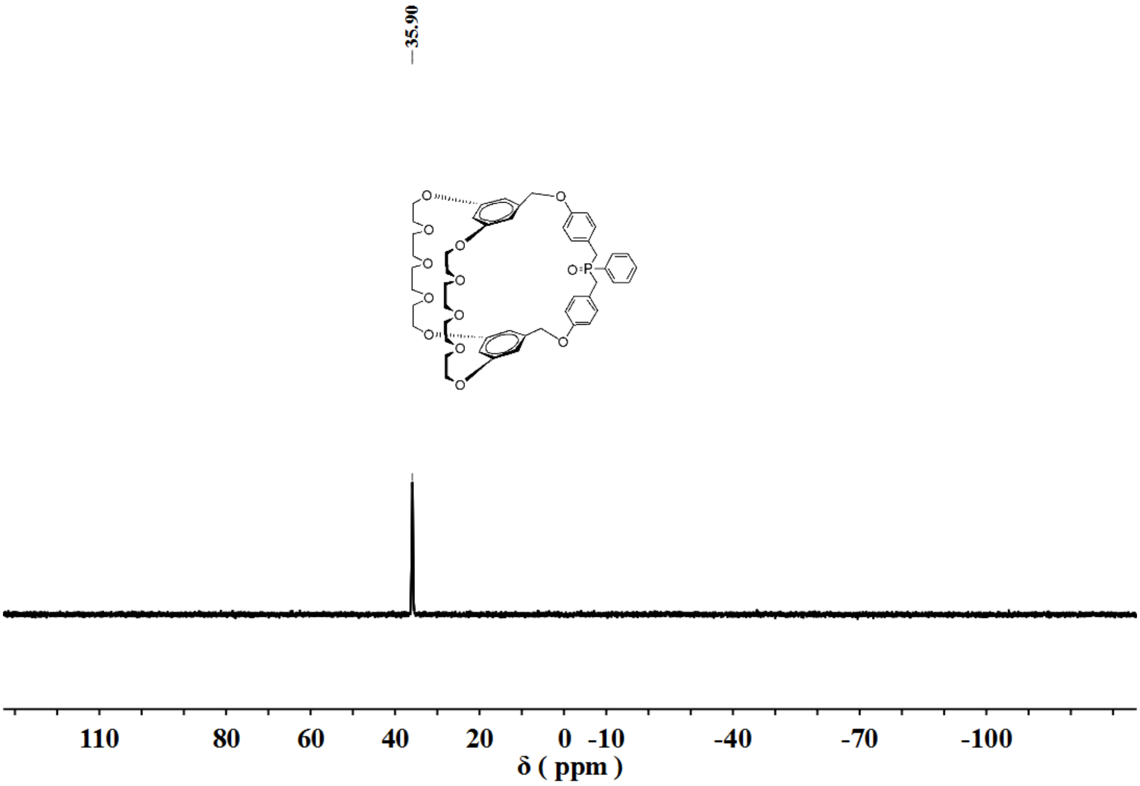


Fig. S25 ^{31}P NMR spectrum (400 MHz, CDCl$_3$, 298 K) of **2**.

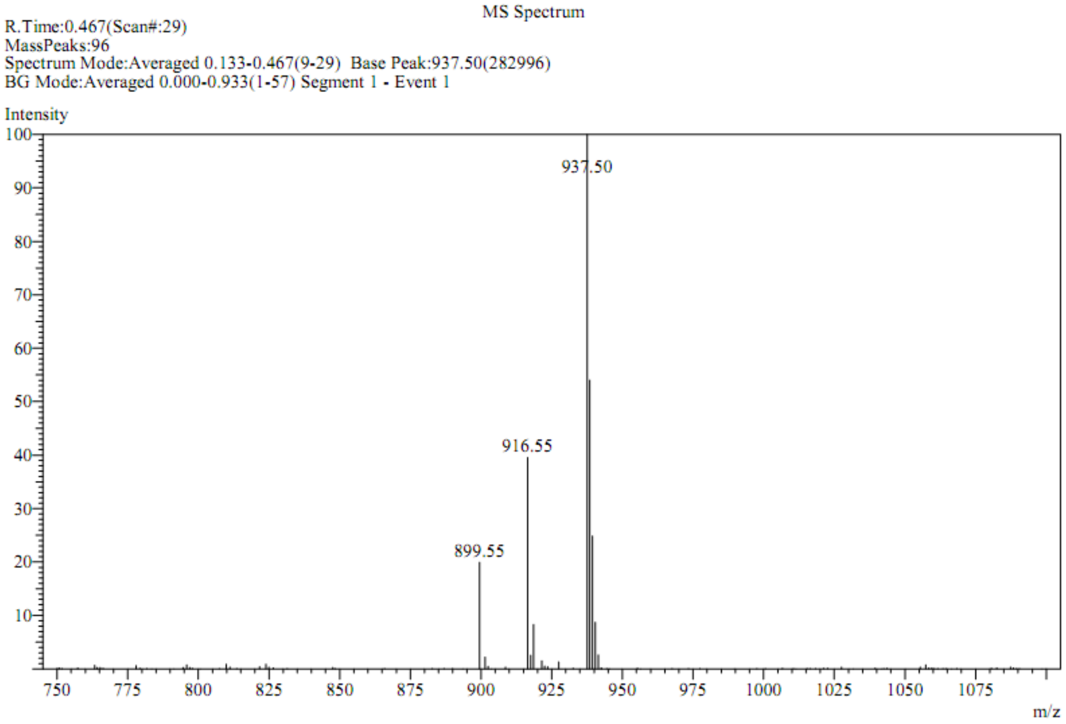


Fig. S26 LR-ESI-MS spectrum of **2**.

3. *Studies of charge transfer interactions by UV-vis spectra*

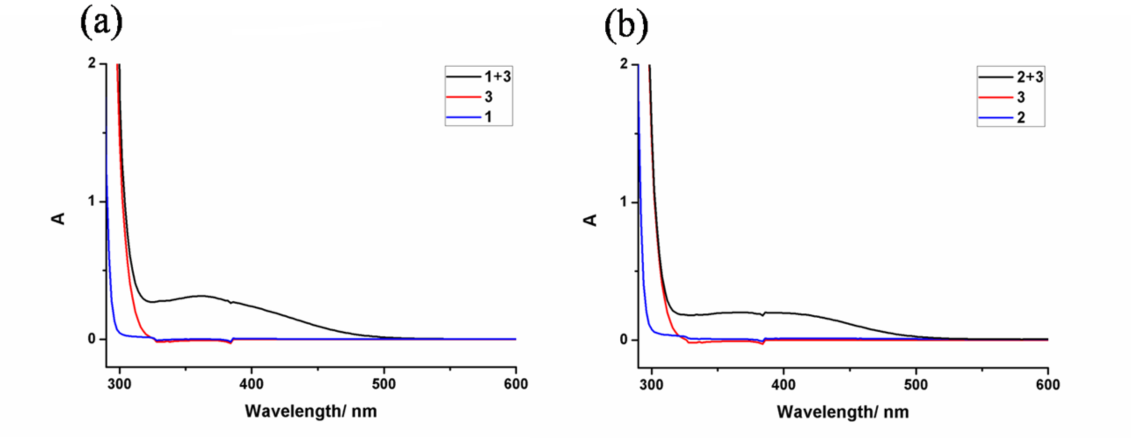


Fig. S27 (a) UV-vis absorption spectra of **1**, **3**, and **1+3** (1:1, molar ratio), respectively in CH_3CN; (b) UV-vis absorption spectra of **2**, **3**, and **2+3** (1:1, molar ratio), respectively in CH_3CN (the concentration for **1**, **2**, and **3** is 8×10^{-4} mM, respectively).

4. *Job plots for the complexes of **1⊃3** and **2⊃3***

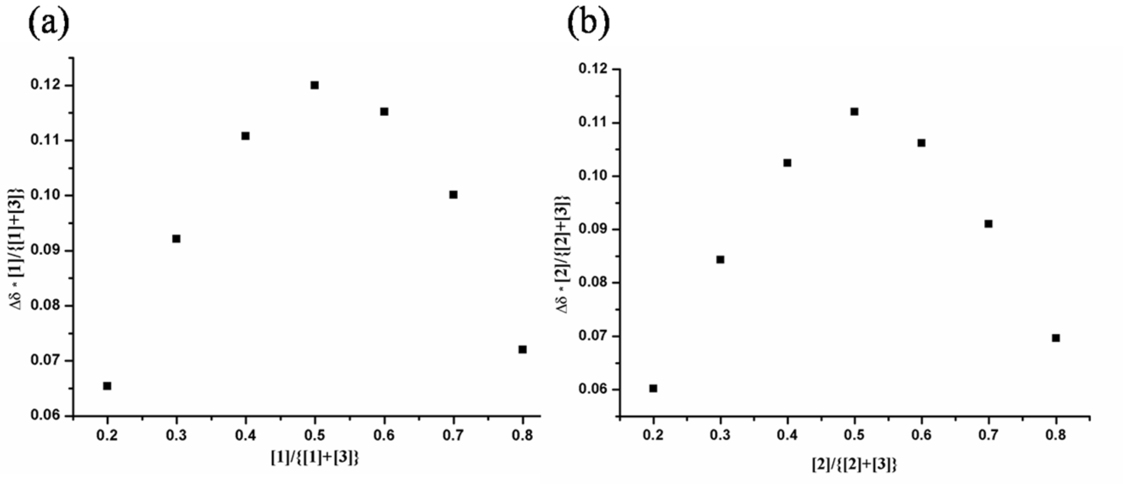


Fig. S28 Job Plots showing the 1:1 stoichiometry of the complexation between **1** and **3** (a) and **2** and **3** (b) in CD_3CN. ([H] + [G] = 4 mM).

5. *LR-ESI-MS spectra of the complexes of **1**⊃**3** and **2**⊃**3***

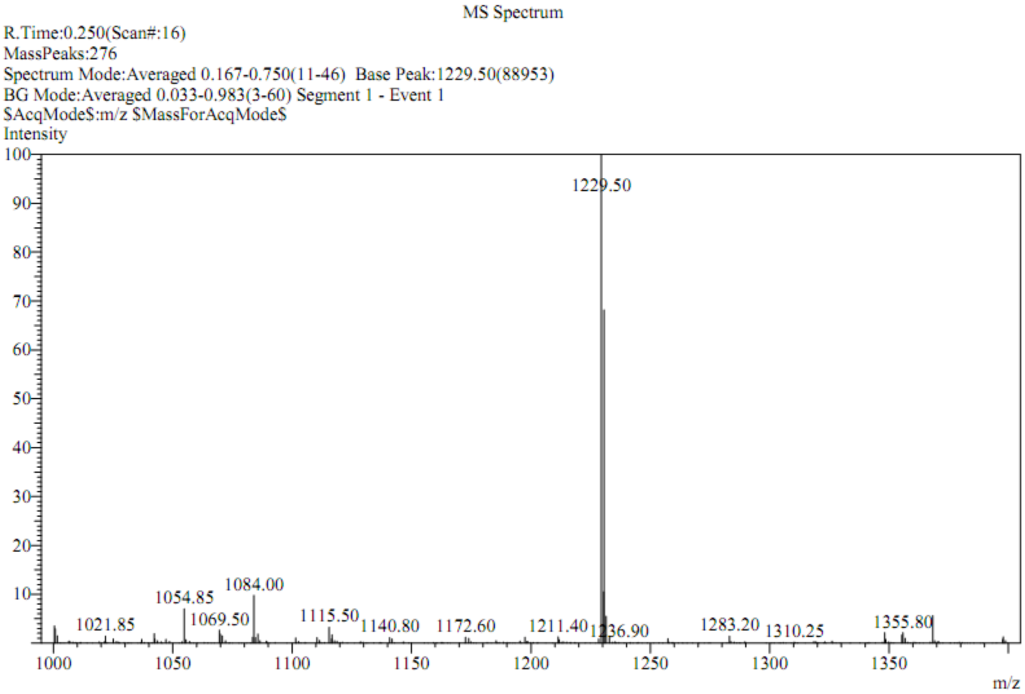


Fig. S29 LR-ESI-MS of an equimolar mixture of **1** and **3**. Assignment of main peaks: *m/z* 1229.50 (100%) for [**1**⊃**3**–PF$_6$]$^+$. This result confirmed the 1:1 complexation stoichiometry between **1** and **3**.

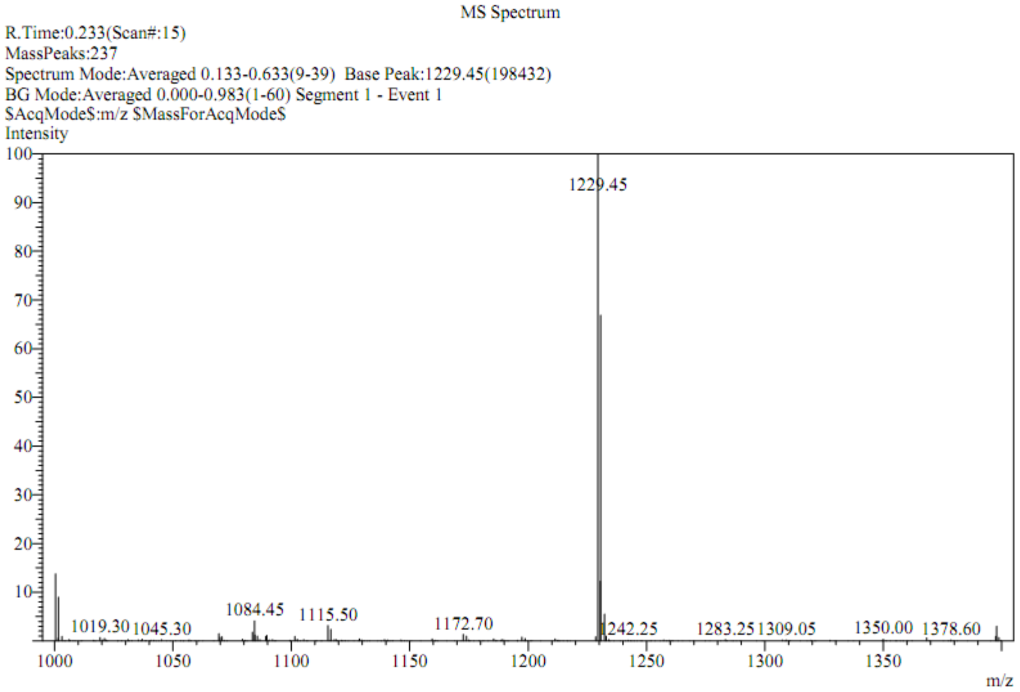


Fig. S30 LR-ESI-MS of an equimolar mixture of **2** and **3**. Assignment of main peaks: *m/z* 1229.45 (100%) for [**2**⊃**3**–PF$_6$] $^+$. This result confirmed the 1:1 complexation stoichiometry between **2** and **3**.

6. *Determination of the association constants of* $\mathbf{1}\supset\mathbf{3}$ *and* $\mathbf{2}\supset\mathbf{3}$ *by* ^1H *NMR*

To determine the association constant between the host (**1** or **2**) and the guest **3**, ^{1}H NMR titration experiments were performed with a constant concentration of the host (2.00 mM) and varying concentrations of the guest. Using a non-linear curve-fitting method, the association constant was obtained for each host-guest combination from the following equation:[S4]

$$\Delta\delta = (\Delta\delta_\infty/[\mathrm{H}]_0)\ (0.5[\mathrm{G}]_0 + 0.5([\mathrm{H}]_0 + 1/K_a) - (0.5\ ([\mathrm{G}]_0^2 + (2[\mathrm{G}]_0(1/K_a - [\mathrm{H}]_0)) + (1/K_a + [\mathrm{H}]_0)^2)^{0.5}))\quad \text{(Eq. S1)}$$

Where $\Delta\delta$ is the chemical shift change of H_a on host at $[G]_0$, $\Delta\delta_\infty$ is the chemical shift change of H_a when the host is completely complexed, $[H]_0$ is the fixed initial concentration of the host, and $[G]_0$ is the initial concentration of the guest.

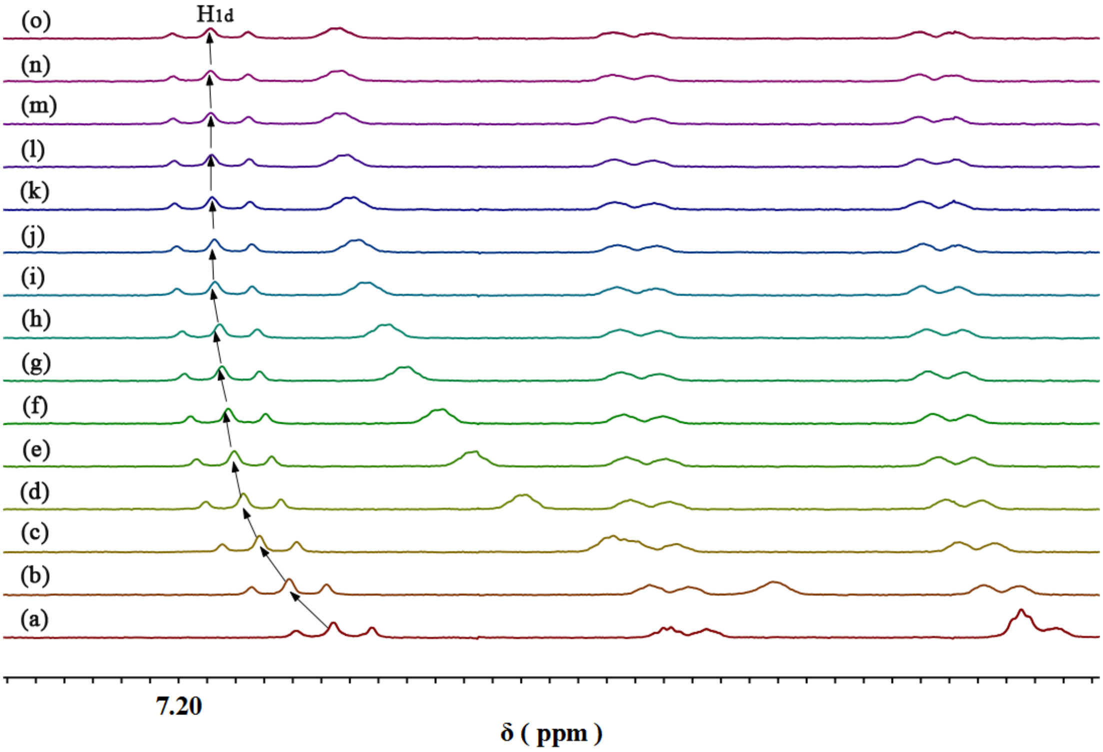


Fig. S31 Partial ^{1}H NMR spectral changes (300 MHz, CD_3CN, 298 K) of **1** at a concentration of 2.00 mM upon addition of **3**: (a) 0.00, (b) 1.00, (c) 2.00, (d) 3.00, (e) 4.00, (f) 5.00, (g) 7.00, (h) 9.00, (i) 13.00, (j) 17.00, (k) 20.00, (l) 24.00, (m) 30.00, (n) 36.00, (o) 40.00 mM.

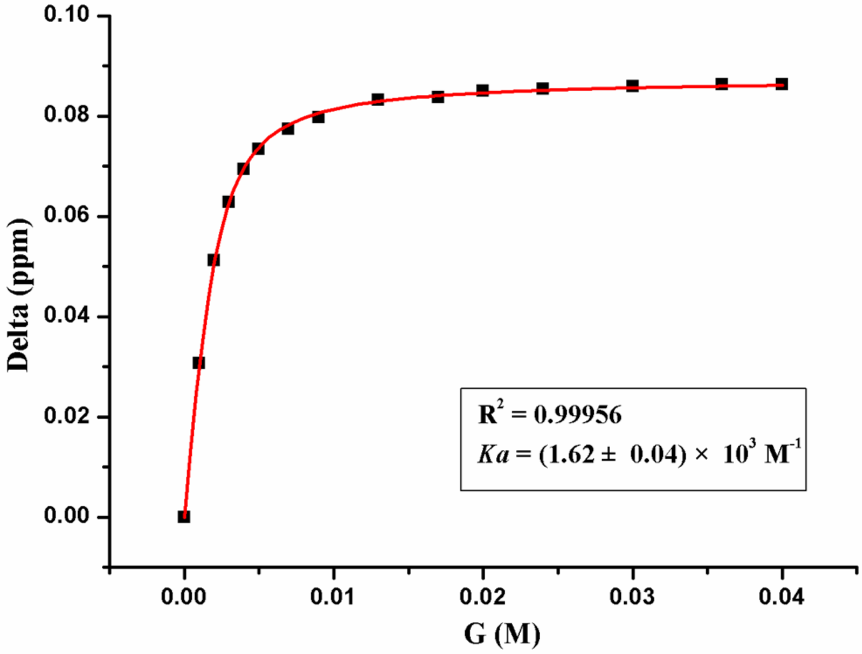


Fig. S32 The chemical shift changes of H_{1d} on **1** upon addition of **3**. The red solid line was obtained from the non-linear curve-fitting using Eq.S1. The association constant (K_a) of **1⊃3** was estimated to be about $(1.62 \pm 0.04) \times 10^3$ M^{-1}.

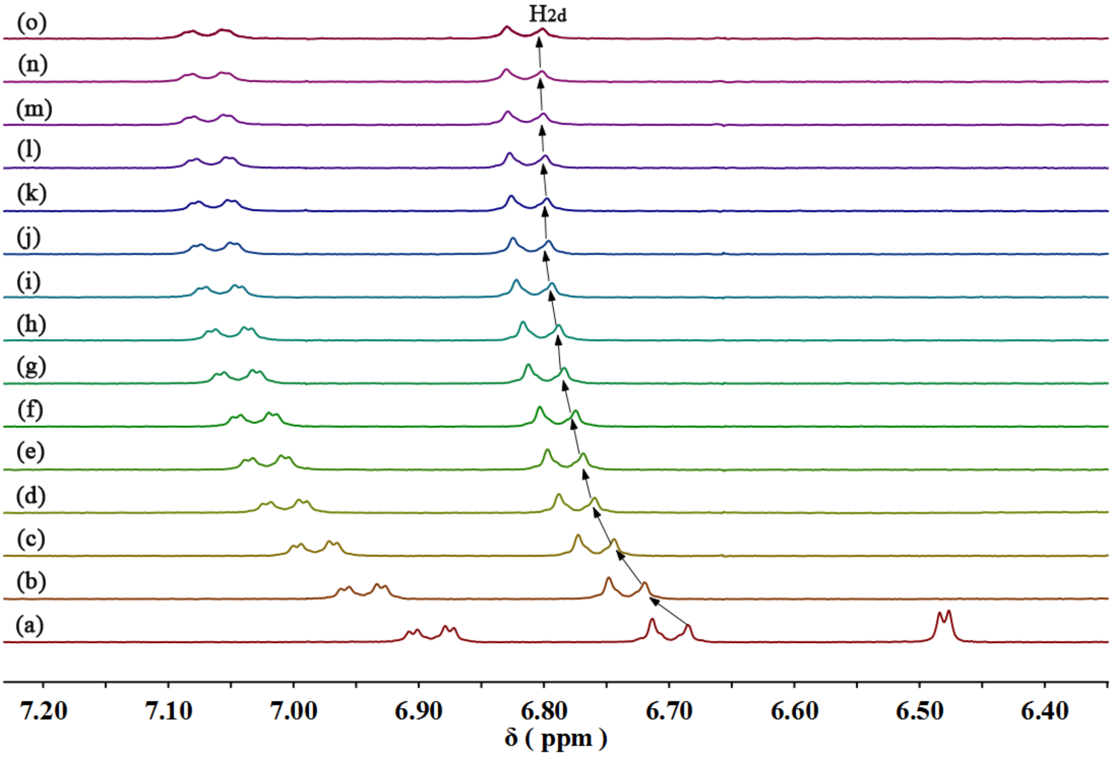


Fig. S33 Partial ^1H NMR spectral changes (300 MHz, CD_3CN, 298 K) of **2** at a concentration of 2.00 mM upon addition of **3**: (a) 0.00, (b) 1.00, (c) 2.00, (d) 3.00, (e) 4.00, (f) 5.00, (g) 7.00, (h) 9.00, (i) 13.00, (j) 17.00, (k) 20.00, (l) 24.00, (m) 30.00, (n) 36.00, (o) 40.00 mM.

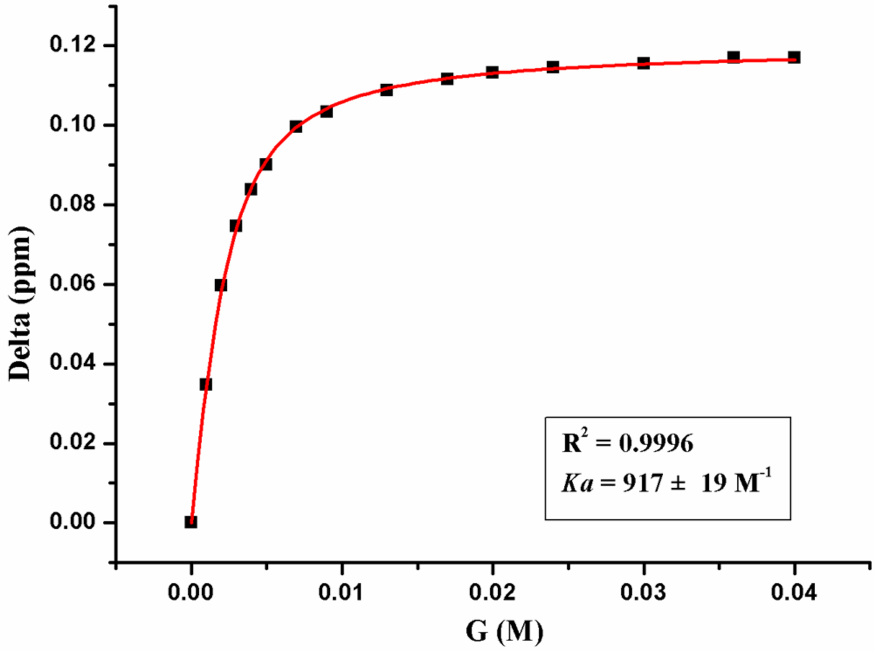


Fig. S34 The chemical shift changes of H_{2d} on **2** upon addition of **3**. The red solid line was obtained from the non-linear curve-fitting using Eq.S1. The association constant (K_a) of **2⊃3** was estimated to be about 917 ± 19 M^{-1}.

7. *Partial 2D COSY NMR spectra of **1** and **1⊃3***

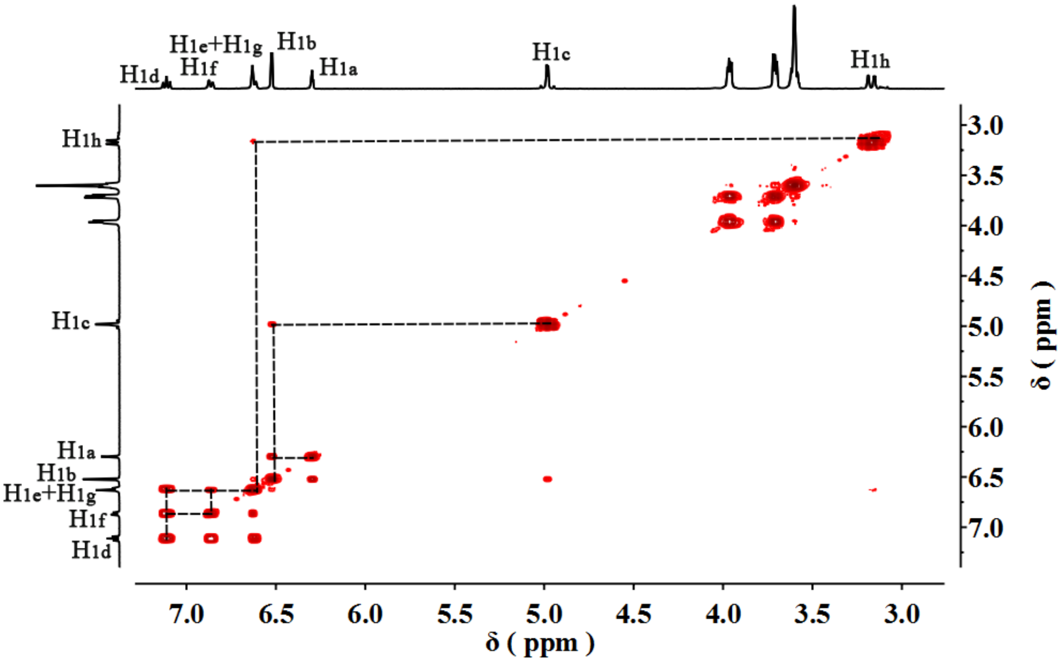


Fig. S35 Partial COSY NMR (400 MHz, CD_3CN, 298 K) spectrum of **1** (6.00 mM).

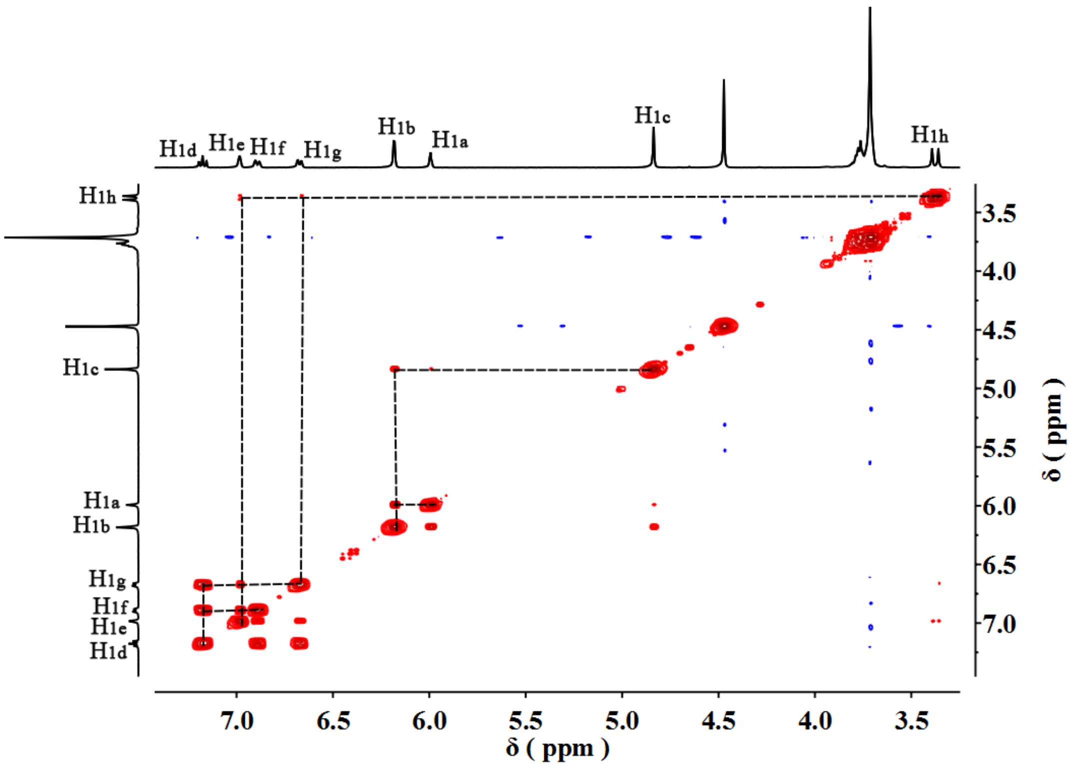


Fig. S36 Partial COSY NMR (400 MHz, CD_3CN, 298 K) spectrum of **1**⊃**3** (1:1, 6.00 mM each).

*8. Partial 2D NOESY NMR spectra of **1⊃3** and **2⊃3***

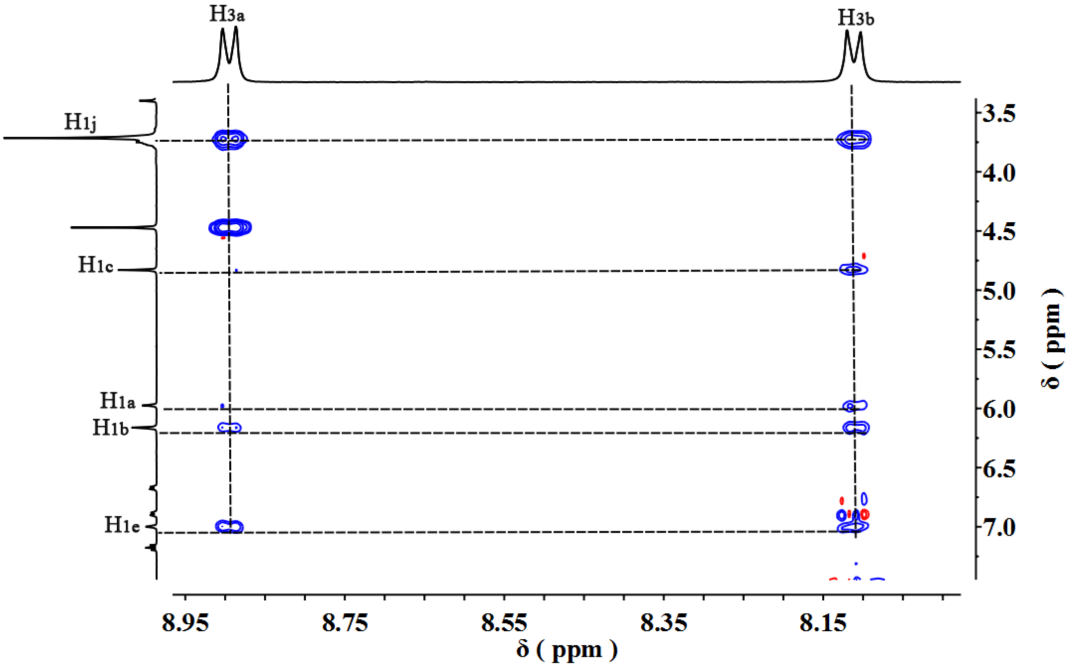


Fig. S37 Partial NOESY NMR (400 MHz, CD_3CN, 298 K) spectrum of **1**⊃**3** (1:1, 6.00 mM each).

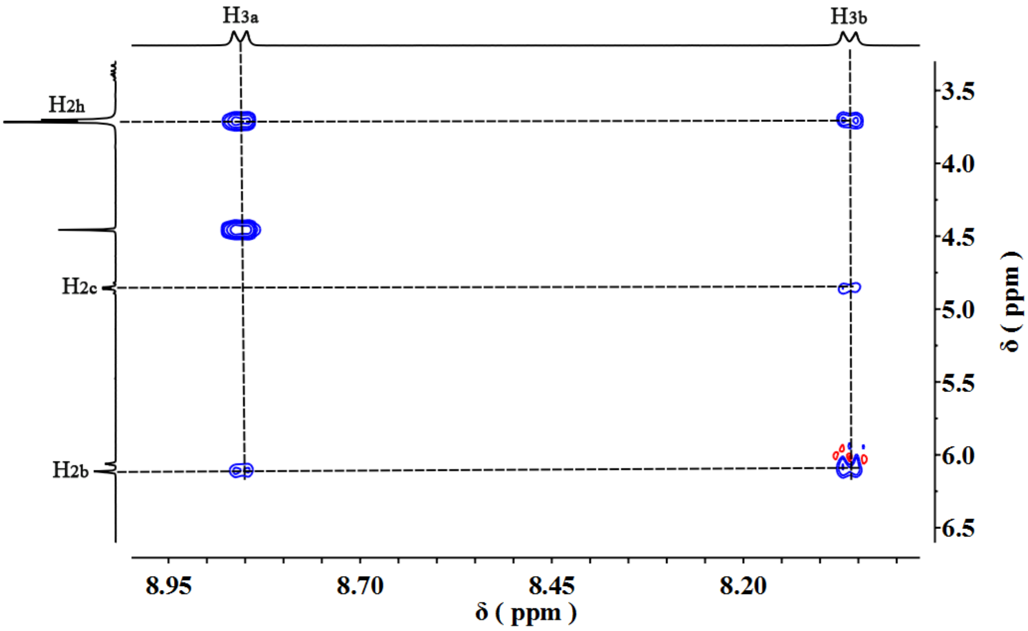


Fig. S38 Partial NOESY NMR (400 MHz, CD_3CN, 298 K) spectrum of **2**⊃**3** (1:1, 6.00 mM each).

*9. X-ray crystal data of **1**⊃3 and **2**⊃3*

Table 1 Crystal data and structure refinement for **1**⊃**3**

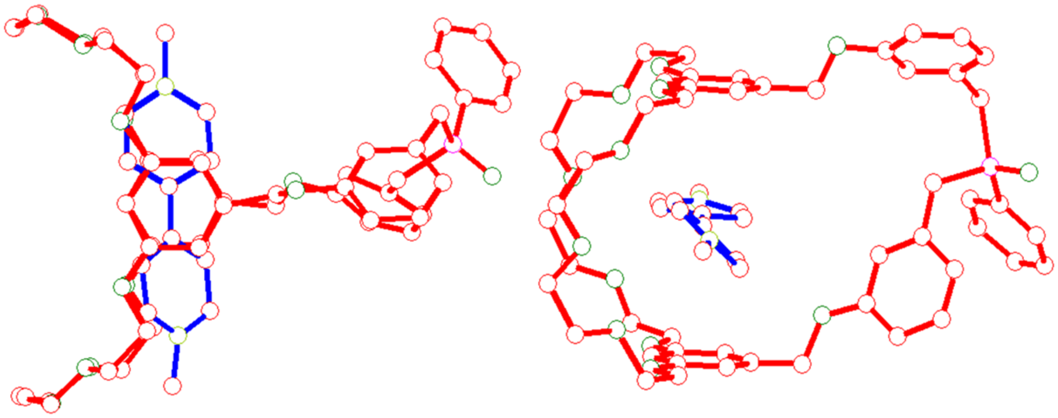
CCDC number	1004105
Empirical formula	$C_{64}H_{80}F_{12}N_3O_{15}P_3$
Formula weight	1452.22
Temperature	173(2)
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	*P2(1)*
a	11.316(2) Å
b	24.717(2) Å
c	14.0638(11) Å
α	90.00°
β	100.065(3)°
γ	90.00°
Volume	3873.0(9) $Å^3$
Z	2
Density (calculated)	1.245
Absorption coefficient	0.164
F(000)	1516
Crystal size	0.28 × 0.24 × 0.22 mm^3

Theta range for data collection	2.21 to 20.61°
Index ranges	−13<=h<=13, −25<=k<=29, −17<=l<=17
Reflections collected	28483
Independent reflections	13314 [R(int) = 0.0191]
Completeness to theta = 26.00°	97.7 %
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on *F*2	1.064
Final R indices [$I > 2\text{sigma}(I)$]	$R1 = 0.0540$, $wR2 = 0.1368$
R indices (all data)	$R1 = 0.0551$, $wR2 = 0.1372$
Largest diff. peak and hole	0.327 and −0.289 e·Å^{-3}

Table 2 Crystal data and structure refinement for **2**⊃**3**

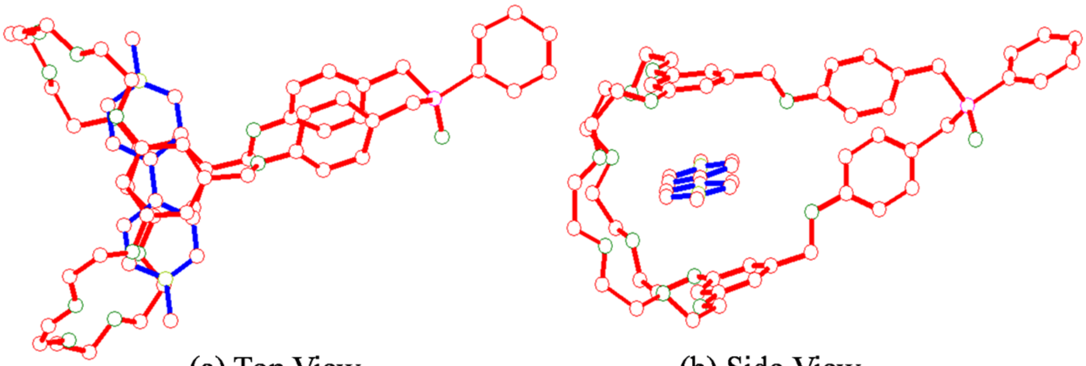
CCDC number	1011981
Empirical formula	$C_{62}H_{73}F_{12}N_3O_{13}P_3$
Formula weight	1375.13
Temperature	296(2)
Wavelength	1.54178 Å
Crystal system	monoclinic
Space group	*P2(1)/n*
a	17.2062(4) Å
b	23.6008(5) Å
c	18.4826(4) Å
α	90.00°
β	90.615(2)°
γ	90.00°
Volume	7505.0(3) Å^3
Z	4
Density (calculated)	1.217
Absorption coefficient	1.468
F(000)	2864
Crystal size	0.28 × 0.26 × 0.22 mm^3
Theta range for data collection	4.45 to 51.08°
Index ranges	−19<=h<=19, −26<=k<=27, −21<=l<=21
Reflections collected	37065
Independent reflections	11403 [R(int) = 0.0437]
Completeness to theta = 63.00°	94.0 %
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on *F*2	1.154
Final R indices [$I > 2\text{sigma}(I)$]	$R1 = 0.1127$, $wR2 = 0.2147$
R indices (all data)	$R1 = 0.1662$, $wR2 = 0.2295$
Largest diff. peak and hole	0.448 and −0.439 e·Å^{-3}

*10. Crystal structures of **1⊃3** and **2⊃3***



(a) Top View (b) Side View

Fig. S39 Crystal structure of **1⊃3** from the top (a) and side view (b). Hydrogen atoms and PF_6^- are omitted for clarity.



(a) Top View (b) Side View

Fig. S40 Crystal structure of **2⊃3** from the top (a) and side view (b). Hydrogen atoms and PF_6^- are omitted for clarity.

References

S1. J. W. Jones, L. N. Zakharov, A. L. Rheingold and H. W. Gibson, *J. Am. Chem. Soc.*, 2002, **124**, 13378.

S2. C. Liu, J. K. Schilling, R. Ravindra, S. Bane and D. G. I. Kingston, *Bioorg. Med. Chem.*, 2004, **12**, 6147.

S3. J. Lee, J.-H. Lee, S. Y. Kim, N. A. Perry, N. E. Lewin, J. A. Ayres and P. M. Blumberg, *Bioorg. Med. Chem.*, 2006, **14**, 2022.

S4. P. R. Ashton, R. Ballardini, V. Balzani, M. Bělohradský, M. T. Gandolfi, D. Philp, L. Prodi, F. M. Raymo, M. V. Reddington, N. Spencer, J. F. Stoddart, M. Venturi and D. J. Williams, *J. Am. Chem. Soc.*, 1996, **118**, 4931.