Supplementary information

Catechol and 1,2,4,5-tetrahydroxybenzene functionalized cyclodiphosphazane ligands synthesis, structural studies, and transition metal complexes

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NMR spectra of compounds 1-16 2–26
HRMS spectra of compounds 1-16 2–26

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Fig. S1 $^{31}\text{P} \{^1\text{H}\}$ NMR spectrum of 1 in CDCl$_3$ (162 MHz)

Fig. S2 $^1\text{H}$ NMR spectrum of 1 in CDCl$_3$ (400 MHz)
Fig. S3 $^{13}$C-$^1$H NMR spectrum of 1 in CDCl$_3$ (101 MHz)

Fig. S4 HRMS spectrum of 1
Fig. S5 $^{31}$P-$^1$H NMR spectrum of 2 in CDCl$_3$(202 MHz)

Fig. S6 $^1$H NMR spectrum of 2 in CDCl$_3$(500 MHz)
Fig. S7 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 2 in CDCl$_3$(126 MHz)
Fig. S8 HRMS spectrum of 2

Fig. S9. The powder-XRD patterns of compound 3. Experimental in blue and simulated in red.
Fig. S10. The powder-XRD patterns of compound 4. Experimental in blue and simulated in red.

Fig. S11. The powder-XRD patterns of compound 5. Experimental in blue and simulated in red. (Some extra peaks observed may be due to the presence of some non-identified material).
Fig. S12 $^{31}\text{P} \{^1\text{H}\}$ NMR spectrum of 6 in CDCl$_3$(162 MHz)

Fig. S13 $^1\text{H}$ NMR spectrum of 6 in CDCl$_3$(500 MHz)
**Fig. S14.** The powder-XRD patterns of compound 6. Experimental in blue and simulated in red.

**Fig. S15** $^{31}$P-$^{1}{_H}$ NMR spectrum of 7 in CDCl$_3$(162 MHz)
Fig. S16 $^1$H NMR spectrum of 7 in CDCl$_3$(500 MHz)

Fig. S17. The powder-XRD patterns of compound 7. Experimental in blue and simulated in red.
**Fig. S18** $^{31}$P-$^1$H NMR spectrum of 8 in CDCl$_3$(162 MHz)

**Fig. S19** $^1$H NMR spectrum of 8 in CDCl$_3$(500 MHz)
**Fig. S20.** The powder-XRD patterns of compound 8. Experimental in black and simulated in red. (Some extra peaks observed may be due to the presence of some non-identified material).

**Fig. S21** $^{31}$P-$^1$H NMR spectrum of 9 in CDCl$_3$(202 MHz)
Fig. S22 $^1$H NMR spectrum of 9 in CDCl$_3$(400 MHz)
Fig. S23 HRMS spectrum of 9
**Fig. S24** $^{31}$P{$\textsuperscript{1}H$} NMR spectrum of 10 in CDCl$_3$(202 MHz)

**Fig. S25** $^1$H NMR spectrum of 10 in CDCl$_3$(500 MHz)
Fig. S26 HRMS spectrum of 10

Fig. S27 $^{31}$P{¹H} NMR spectrum of 11 in CDCl$_3$(202 MHz)
Fig. S28 $^1$H NMR spectrum of 11 in CDCl$_3$(400 MHz)
Fig. S29 HRMS spectrum of 11

Fig. S30 $^{31}$P{¹H} NMR spectrum of 12 in CDCl$_3$(202 MHz)
Fig. S31 $^1$H NMR spectrum of 12 in CDCl$_3$(500 MHz)

Fig. S32 HRMS spectrum of 12
Fig. S33 $^{31}$P-$^1$H NMR spectrum of 13 in CDCl$_3$(202 MHz)

Fig. S34 $^1$H NMR spectrum of 13 in CDCl$_3$(500 MHz)
Fig. S35 HRMS spectrum of 13

Fig. S36 $^{31}$P{¹H} NMR spectrum of 14 in CDCl₃(202 MHz)
Fig. S37 $^1$H NMR spectrum of 14 in CDCl$_3$(500 MHz)

Fig. S38 HRMS spectrum of 14
Fig. S39 $^{31}$P{${}^1$H} NMR spectrum of 15 in CDCl$_3$(202 MHz)

Fig. S40 $^1$H NMR spectrum of 15 in CDCl$_3$(500 MHz)
Fig. S41 HRMS spectrum of 15

Fig. S42 $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of 16 in CDCl$_3$(202 MHz)
Fig. S43 $^1$H NMR spectrum of 16 in CDCl$_3$(500 MHz)