Supporting Information

2-Aminophenolate Ligands for Phosphorus(V): A Lithium Salt Featuring the Chiral $[\text{P(OC}_6\text{H}_4\text{NR)}_3]^{-}$ Anion

Chuantian Zhan, Zeyu Han, Brian O. Patrick and Derek P. Gates*

Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, British Columbia, Canada, V6T 1Z1. E-mail: dgates@chem.ubc.ca

Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2018

Fig. S1 The minor component (7%) in the molecular structure for intermediate 3a (thermal ellipsoids are displayed at 50% probability level). Hydrogen atoms are omitted for clarity. Bond lengths and angles are similar to those found in the major structure.
Fig. S2 $^{31}$P$[^1]H$ NMR spectra (121 MHz, CDCl$_3$, 298 K) of phosphoranes 2a-c and intermediate 3a.
Fig. S3 $^1$H NMR spectra (300 MHz, CDCl$_3$, 298 K) of phosphoranes: (a) 2a; (b) 2b; (c) 2c; (d) 3a recrystallized from CH$_2$Cl$_2$ (* indicates the residual CHCl$_3$ and † indicates the residual CH$_2$Cl$_2$ solvent).

Fig. S4 $^{13}$C($^1$H) NMR spectrum (100.5 MHz, CD$_2$Cl$_2$, 298 K) of phosphorane 2a (* indicates the solvent).
Fig. S5 $^{19}$F($^1$H) NMR spectrum (282 MHz, CDCl$_3$, 298 K) of phosphorane 2c.

Fig. S6 $^1$H NMR spectra (400 MHz, DMSO-$d_6$, 298 K) of Li(THF)$_3$-[4a] (* indicates the solvent).
Fig. S7 $^1$H($^{31}$P) NMR spectra (400 MHz, DMSO-$d_6$, 298 K) of Li(THF)$_3$ fac-[4a].
Fig. S8 $^{13}$C[1H] NMR spectra (100.5 MHz, DMSO-d$_6$, 298 K) of Li(THF)$_3$ [4a] (* indicates the solvent).
Fig. S9 $^1$H-$^{13}$C HSQC NMR spectrum (400 MHz for $^1$H, DMSO-$d_6$, 298 K) of Li(THF)$_3$fac-[4a] (The ordinate axis shows the $^{13}$C[$^1$H] NMR spectrum and the abscissa axis shows the $^1$H NMR spectrum; * indicates the solvent).
Fig. S10 $^1$H–$^{13}$C HMBC NMR spectrum (400 MHz for $^1$H, DMSO–$d_6$, 298 K) of Li(THF)$_3$–fac–[4a] (The ordinate axis shows the $^{13}$C–$^1$H NMR spectrum and the abscissa axis shows the $^1$H NMR spectrum; * indicates the solvent).
Fig. S11 $^{31}$P NMR spectrum (121 MHz, 298 K) of Li(THF)$_3$ fac-[4a] in DMSO-$d_6$ over 6 months.

Fig. S12 $^1$H-$^{31}$P HMBC NMR spectrum (400 MHz for $^1$H, DMSO-$d_6$, 298 K) of Li(THF)$_3$ fac-[4a] (The ordinate axis shows the $^{31}$P-$^1$H NMR spectrum and the abscissa axis shows the $^1$H NMR spectrum).
Fig. S13 Partial $^1$H-$^{31}$P HMBC NMR spectrum (400 MHz for $^1$H, DMSO-$d_6$, 298 K) of Li(THF)$_3$fac–[4a] (The ordinate axis shows the $^{31}$P[$^1$H] NMR spectrum and the abscissa axis shows the $^1$H NMR spectrum).
Fig. S14 Partial $^1$H-$^{31}$P HMBC NMR spectrum (400 MHz for $^1$H, DMSO-$d_6$, 298 K) of Li(THF)$_3$fac-[4a] (The ordinate axis shows the $^{31}$P($^1$H) NMR spectrum and the abscissa axis shows the $^1$H NMR spectrum).