Di-, tri- and tetraphosphine-substituted Fe/Se carbonyls: Synthesis, Characterization and electrochemical properties

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Figure S2. $^1$H NMR (500 MHz, CDCl$_3$, 25°C) spectrum of 1. Assignments: $\delta =$ 7.47-6.97 (m, 20H, 4C$_6$H$_5$), 1.87 (t, $^2J_{P-H} = 4.5$ Hz, 12H, 4CH$_3$) ppm.
Figure S3. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 1.  
Assignments: $\delta = 11.28$ (s) ppm

Figure S4. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 1.  
Assignments: $\delta = 212.3$ (t, $^2J_{P-C} = 21.4$, Fe(CO)$_2$), 139.8-125.3 (CsHs), 14.7 (t, $J_{P-C} = 17.4$ Hz, PCH$_3$) ppm
Figure S5. FT-IR (CH$_2$Cl$_2$, 25°C) spectrum of 2. Assignments: $\nu_{CO} = 2000, 1946$ cm$^{-1}$.

Figure S6. $^1$H NMR (500 MHz, CDCl$_3$, 25°C) spectrum of 2. Assignments: $\delta = 7.65, 7.14, 7.08$ (d, t, $^3J_{H-H} = 7.5$ Hz, 10H, 2C$_6$H$_5$), 1.58 (t, $^2J_{P-H} = 4$Hz, 18H, 6CH$_3$) ppm.
Figure S7. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 2. 

Assignments: $\delta = 2.04$ (s) ppm

Figure S8. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 2. Assignments: $\delta = 212.7$ (t, $^{2}J_{P-C} = 22.0$, Fe(CO)$_2$), 136.7, 133.6, 128.1, 125.6 (C$_6$H$_5$), 17.4 (t, $^{3}J_{P-C} = 16.2$ Hz, PCH$_3$) ppm.
Figure S9. FT-IR (CH$_2$Cl$_2$, 25°C) spectrum of 3-anti.

Figure S10. $^1$H NMR (500 MHz, CDCl$_3$, 25 °C) spectrum of 3-anti.

Assignments: $\delta$ = 7.48-6.86 (m, 20H, 4C$_6$H$_5$), 3.50, 2.63 (2s, 4H, 2PhCH$_2$), 1.71 (t, $J = 8.0$ Hz, 12H, 4PCH$_3$) ppm.
Figure S11. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 3-anti.

**Assignments:** $\delta = 216.7$, (t, $^2J_{P-C} = 3.2$ Hz, PFe(CO)$_2$), 126.0-141.6 (m, C$_6$H$_5$), 32.0 (s, Ph$_2$H), 20.9 (d, $^1J_{P-C} = 12.8$ Hz, PCH$_3$), 20.7 (d, $^1J_{P-C} = 11.9$ Hz, PCH$_3$).

Figure S12. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 3-anti.

**Assignments:** $\delta = 216.7$, (t, $^2J_{P-C} = 3.2$ Hz, PFe(CO)$_2$), 126.0-141.6 (m, C$_6$H$_5$), 32.0 (s, Ph$_2$H), 20.9 (d, $^1J_{P-C} = 12.8$ Hz, PCH$_3$), 20.7 (d, $^1J_{P-C} = 11.9$ Hz, PCH$_3$).
Figure S13. VT-\textsuperscript{1}HNMR spectrum of 3-anti in CD\textsubscript{2}Cl\textsubscript{2}.

Figure S14. VT-\textsuperscript{31}PNMR spectra of 3-anti in CD\textsubscript{2}Cl\textsubscript{2}.
Figure S15. FT-IR (CH$_2$Cl$_2$, 25°C) spectrum of 3-syn.
Assignments: $\nu_{CO} = 1977, 1932, 1912$ cm$^{-1}$.

Figure S16. $^1$H NMR (500 MHz, CDCl$_3$, 25°C) spectrum of 3-syn.
Assignments: $\delta = 7.41-7.10$ (m, 20H, 4C$_6$H$_5$), 3.27 (s, 4H, 2PhCH$_2$), 1.56 (d, $J = 6.5$ Hz, 12H, 4PCH$_3$) ppm.
Figure S17. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 3-syn.

*Assignments*: $\delta = 21.58$ (s) ppm

Figure S18. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 3-syn.

*Assignments*: $\delta = 217.8$, (t, $^2J_{P-C} = 3.2$ Hz, PFe(CO)$_2$), 126.5-142.5 (m, C$_6$H$_5$), 30.3 (s, PhCH$_2$), 20.5, 20.3 (2t, $J_{P-C} = 11.2$ Hz, PCH$_3$).
Figure S19. FT-IR (in CH₂Cl₂, 25°C) spectrum of 4-anti.
Assignments: ν\textsubscript{CO} = 1974, 1937, 1906 cm\(^{-1}\).

Figure S20. \(^1\)H NMR (500 MHz, CDCl₃, 25 °C) spectrum of 4-anti. Assignments: δ = 7.14-7.41(m, 10H, 2C₆H₅), 3.65, 3.13 (2s, 4H, 2CH₂), 1.39 (d, \(^2\)Jₚ-H = 8.5Hz, 18H, 6CH₃) ppm.
Figure S21. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 4-anti. 
*Assignments:* $\delta = 21.02$ (s) ppm.

Figure S22. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 4-anti. 
*Assignments:* $\delta = 217.2$ (t, $^2J_{P\text{-}C} = 18.9$, Fe(CO)$_2$), 141.8-125.7 (m, C$_6$H$_5$), 31.6 (s, CH$_2$), 22.0 (d, $J_{P\text{-}C} = 27.7$ Hz, PCH$_3$) ppm.
Figure S23. FT-IR (in CH₂Cl₂, 25°C) spectrum of 4-syn.
Assignments: νCO = 1975, 1929, 1908 cm⁻¹.

Figure S24. ¹H NMR (500 MHz, CDCl₃, 25 °C) spectrum of 4-syn.
Assignments: δ = 7.17-7.32 (m, 10H, 2C₆H₅), 3.67 (s, 4H, 2PhCH₂), 1.31 (d, J = 4.5 Hz, 18H, 6CH₃) ppm
Figure S25. $^{31}$P NMR (202 MHz, CDCl$_3$, 25 °C) spectrum of 4-syn. Assignments: $\delta = 10.35$ (s) ppm

Figure S26. $^{13}$C NMR (126 MHz, CDCl$_3$, 25 °C) spectrum of 4-syn. Assignments: $\delta = 218.4$ (t, $^2J_{P-C} = 3.7$, Fe(CO)$_2$), 141.4, 128.8, 128.4, 126.5 (s, C$_6$H$_5$), 30.1 (s, CH$_2$), 22.1-21.7 (m, PCH$_3$).
Figure S27  $^{31}$P NMR spectra in the reaction of 5 equivalents of PMe$_3$ with Fe(μ-SeCH$_2$Ph)$_2$(CO)$_6$ in toluene (stirred at room temperature for 4h (1), then heated to 100°C for 1h (2)).

Figure S28. FT-IR (in CH$_2$Cl$_2$, 25°C) spectrum of 5. Assignments: $\nu_{CO} = 1942$, 1885, 1660 cm$^{-1}$. 
Figure S29. $^1$H NMR (500 MHz, C$_6$D$_6$, 25 °C) spectrum of 5. *Assignments:* $\delta =$ 6.91-7.65 (m, 25H, 4C$_6$H$_5$), 3.99, 3.55, 3.15, 2.90 (ABq, $^2J_{H-H} = 11.5$Hz, 4H, 2C$_6$H$_5$CH$_2$), 1.81, 1.63, 1.56, 1.51, 1.29, 1.09 (6d, $^2J_{P-H} = 8.0$ Hz, 18H, 6CH$_3$) ppm.

Figure S30. $^{31}$P NMR (202 MHz, C$_6$D$_6$, 25 °C) spectrum of 5. *Assignments:* $\delta =$ 32.0 (d, $J = 11.7$ Hz, *apical-*Fe(CO)(PPhMe$_2$)$_2$), 29.6 (d, $J = 11.6$ Hz, *apical-*Fe(CO)$_2$PPhMe$_2$), 17.9 (t, $J = 12.1$ Hz, *basal-*Fe(CO)(PPhMe$_2$)$_2$) ppm.
Figure S31. $^{13}$C NMR (126 MHz, C$_6$D$_6$, 25 °C) spectrum of 5. Assignments: $\delta =$ 221.8-222.2 (m, Fe(CO)), 217.6 (s, Fe(CO)), 143.9-125.8 (m, C$_6$H$_5$), 31.4(s, CH$_2$), 23.9-15.7 (m, PCH$_3$) ppm.

Figure S32. FT-IR (in CH$_2$Cl$_2$, 25°C) spectrum of 6.
Assignments: $\nu$co = 1938, 1880, 1855 cm$^{-1}$. 
Figure S33. $^1$H NMR (500 MHz, C$_6$D$_6$, 25 °C) spectrum of 6. Assignments: $\delta = 6.95$-$7.60$ (m, 10H, 2C$_6$H$_5$), 4.01, 3.75 (2d, $^2$J$_{H-H} = 11.5$Hz, 2H, e-C$_6$H$_5$CH$_2$), 3.15 (s, 2H, a-C$_6$H$_5$CH$_2$), 1.27, 1.22, 1.18 (3d, $^2$J$_{P-H} = 8.0$ Hz, 27H, 9CH$_3$) ppm.

Figure S34. $^{31}$P NMR (202 MHz, C$_6$D$_6$, 25 °C) spectrum of 6. Assignments: $\delta = 22.0$ (d, $^3$J$_{P-P} = 11.5$ Hz, apical-Fe(CO)(PMe$_3$)$_2$), 19.9 (d, $^3$J$_{P-P} = 8.7$ Hz, apical-Fe(CO)$_2$PMe$_3$), 22.0 (dd, $^3$J$_{P-P} = 11.3$, 9.1Hz, basal-Fe(CO)(PMe$_3$)$_2$).
Figure S35. $^{13}$C NMR (126 MHz, C$_6$D$_6$, 25 °C) spectrum of 6. Assignments: $\delta =$ 221.3-222.8 (m, Fe(CO)), 218.2 (s, Fe(CO)), 143.1-125.8 (m, C$_6$H$_5$), 31.3 (s, CH$_2$), 24.2-15.5 (m, PCH$_3$) ppm.
Figure S36. FT-IR (in toluene, 25°C) spectrum of 7. Assignments: $\nu_{CO} = 1938, 1880, 1855 \text{ cm}^{-1}$.

Figure S37. $^1$H NMR (500 MHz, C$_6$D$_6$, 25°C) spectrum of 7. Assignments: $\delta = 6.96$-$7.79$ (m, 10H, 2C$_6$H$_5$), 3.67 (d, 2H, e-C$_6$H$_3$CH$_2$), 3.15 (s, 2H, a-C$_6$H$_3$CH$_2$), 1.09-$1.45$ (m, 36H, 12CH$_3$) ppm.
Figure S38. $^{31}$P NMR (202 MHz, C$_6$D$_6$, 25 °C) spectrum of 7. Assignments: $\delta = 26.6$ (s), 24.1 (s), 13.1 (s), 10.0 (s).

Figure S39. Plots of $i_{\text{cat}}$ (μA) vs [HOAc] (mM) for a solution of 4, 6 and 7 (1.0 mM) with 0.1 M n-Bu$_4$NPF$_6$/MeCN at a scan rate of 0.1 V s$^{-1}$. 
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Table S2. Crystal data and structure refinement parameters for compounds 4-7.

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Table S3
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Table S4
Selected bond lengths (Å) and angles (°) for 2.

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Table S5
Selected bond lengths (Å) and angles (°) for 3-syn.

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Table S6
Selected bond lengths (Å) and angles (º) for 3-anti.
Table S7

Selected bond lengths (Å) and angles (°) for 4-syn.

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Table S8

Selected bond lengths (Å) and angles (°) for 4-anti.

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Selected bond lengths (Å) and angles (º) for 5.

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Table S10
Selected bond lengths (Å) and angles (º) for 6.

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Table S11
Selected bond lengths (Å) and angles (º) for 7.

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