Supporting information

Facile Preparation of Scandium Terminal Imido Complex with Phosphazene Ligand

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Figure S1. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **1**.

Figure S2. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

Figure S3. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

Figure S4. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

Figure S5. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

Figure S6. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

Figure S7. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

Figure S8. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **4**.

Figure S9. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **4**.

Figure S10. ^{1}H NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

Figure S11. ^{31}P NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

Figure S12. ^{13}C NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

Figure S13. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

Figure S14. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

Figure S15. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

Figure S16. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **9** on heating at 60 ^{o}C for 12 h.

Figure S17. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of ligand HL^2 {$HN[Ph_2PNC_6H_3(^iPr)_2]_2$}.

Figure S18. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **9** with 2 equivalent of DMAP at 25 ^{o}C for 12 h.

Figure S19. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **9** with 2 equivalent of DMAP at 25 ^{o}C for 12 h.

Figure S20. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

Figure S21. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

Figure S22. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

Figure S23. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **10** on heating at 100 ^{o}C for 12 h.

Figure S24. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **10** with 2 equivalent of DMAP at 80 ^{o}C for 5 h.

Figure S25. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **10** with 2 equivalent of DMAP at 80 ^{o}C for 5 h.

Figure S26. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **11**.

Figure S27. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **11**.

Figure S28. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **12**.

Figure S29. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **12**.

Figure S30. X-ray structure of **10** with 35% probability of thermal ellipsoids.

Table S1. Crystallographic data and structure refinement details for complexes **4, 9, 10** and **11.**

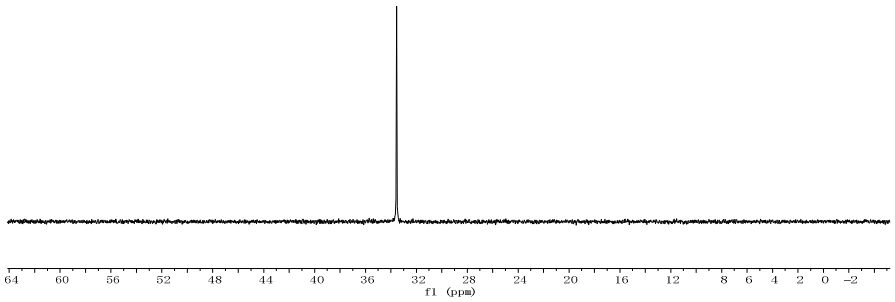

Figure S1. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **1**.

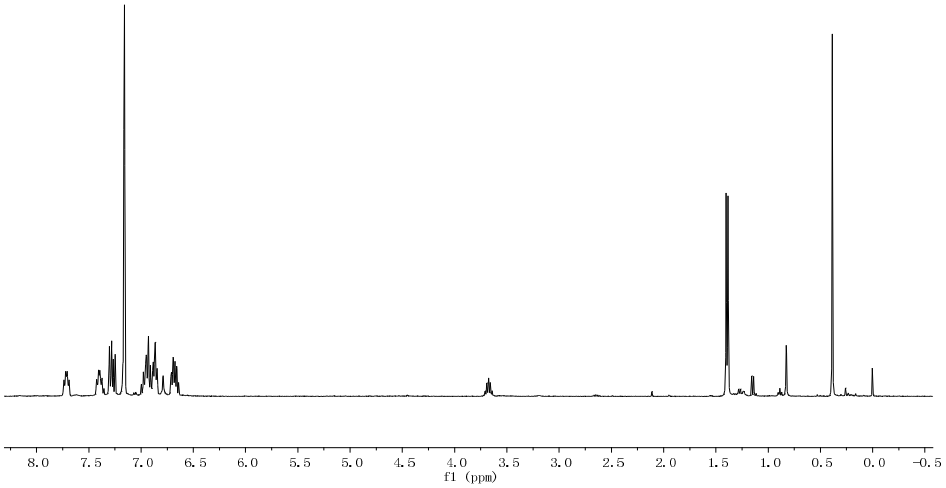

Figure S2. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

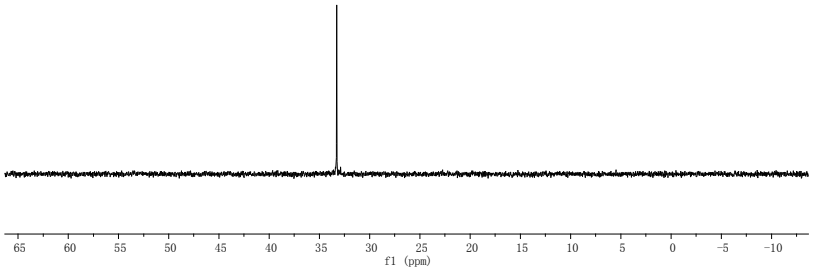

Figure S3. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

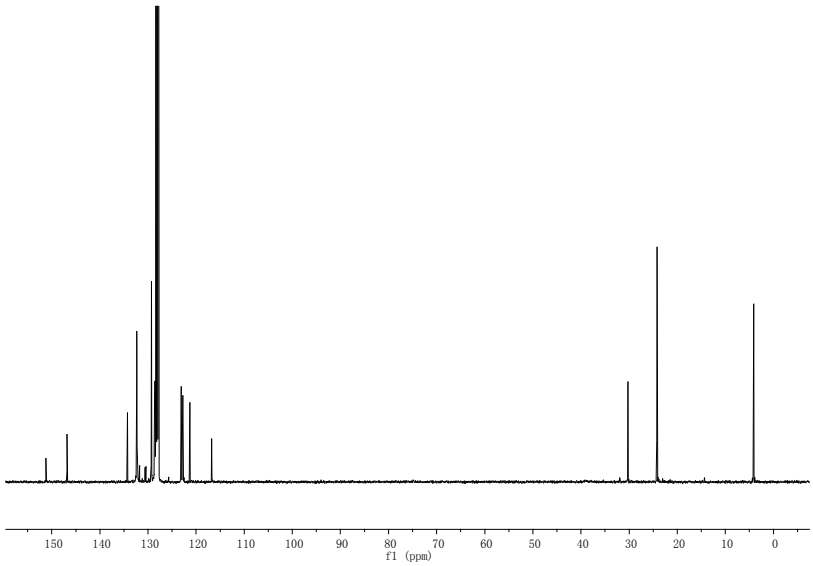

Figure S4. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **2**.

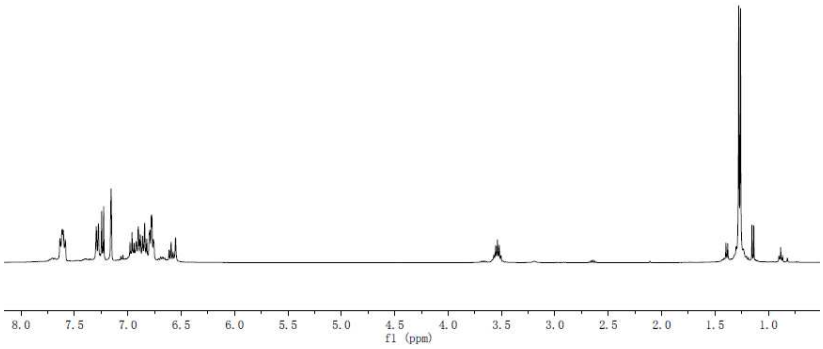

Figure S5. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

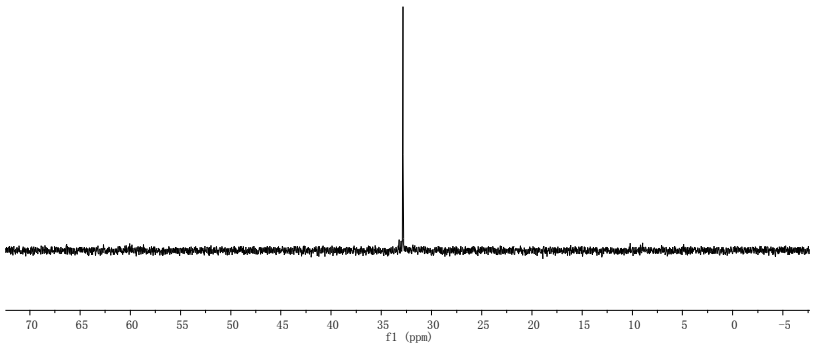

Figure S6. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

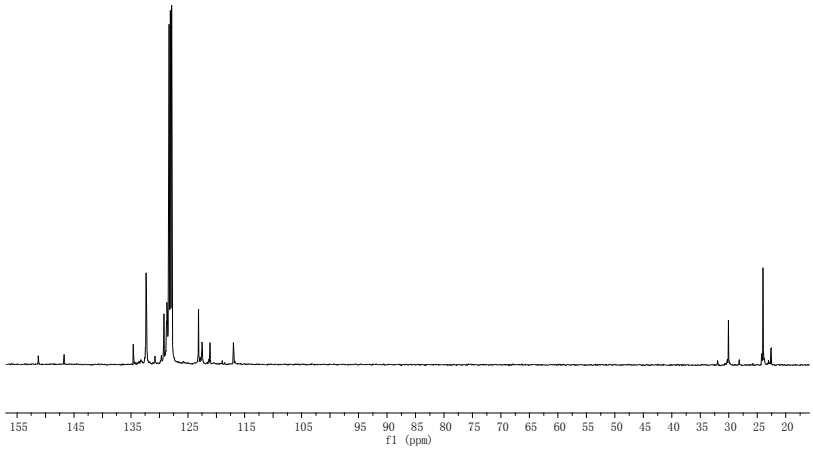

Figure S7. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **3**.

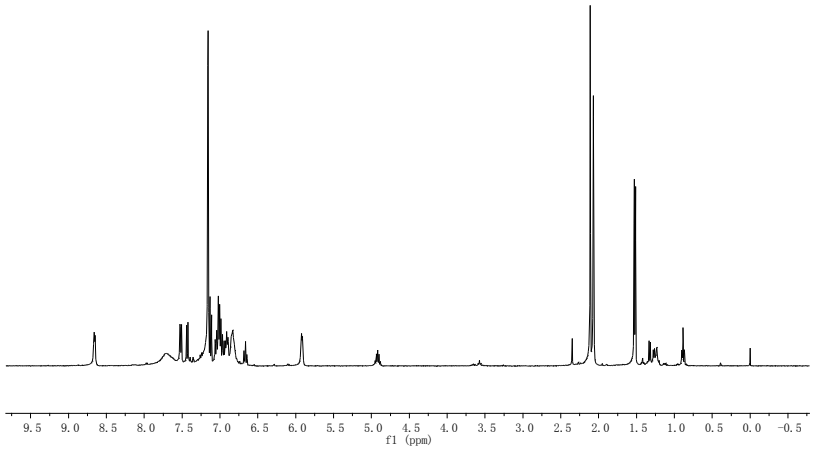

Figure S8. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **4**.

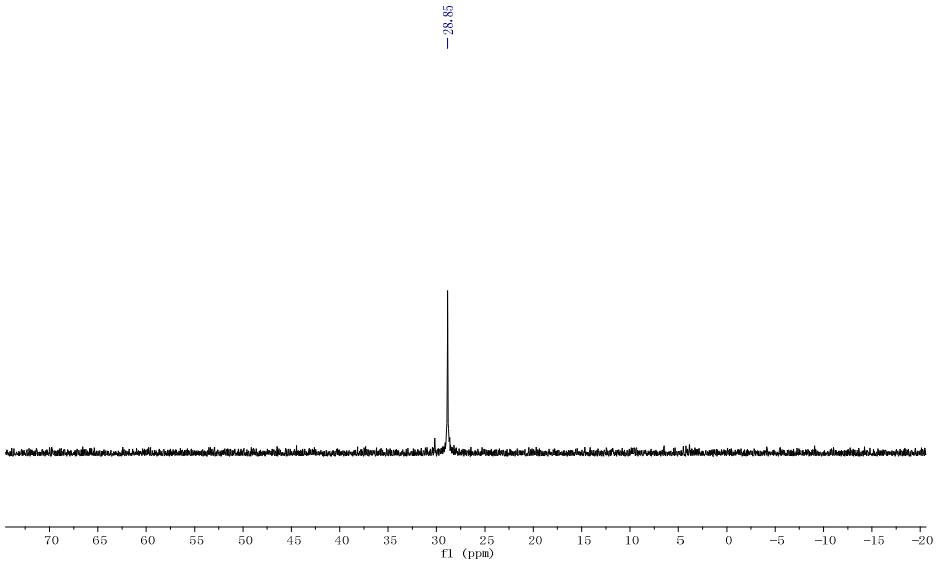

Figure S9. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **4**.

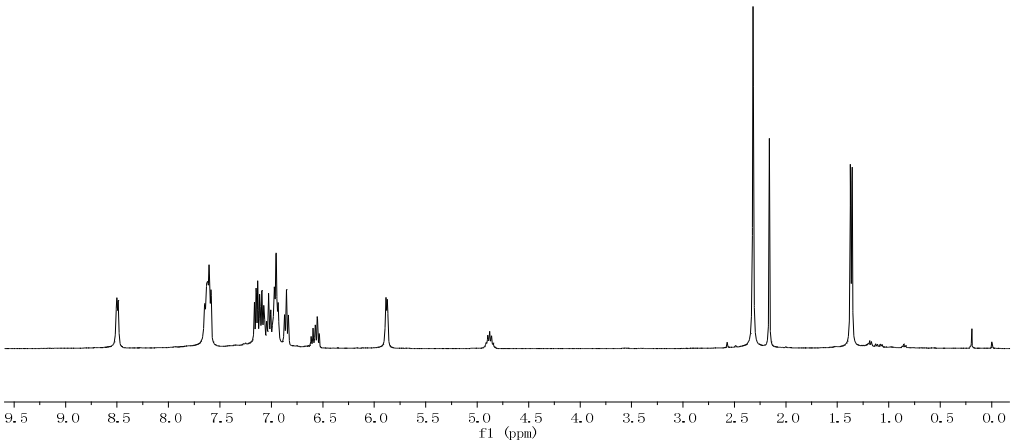

Figure S10. ^{1}H NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

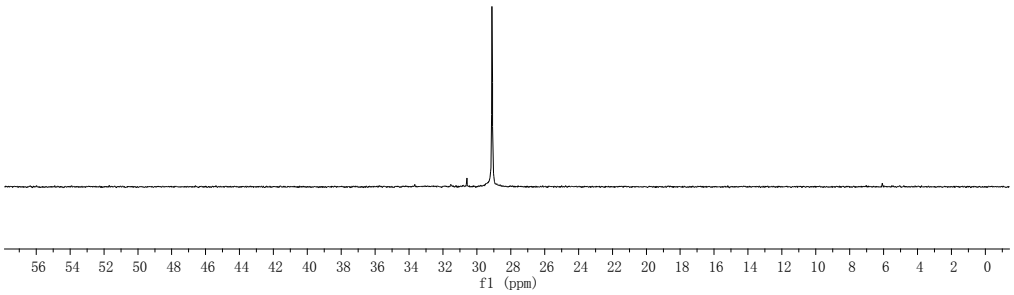

Figure S11. ^{31}P NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

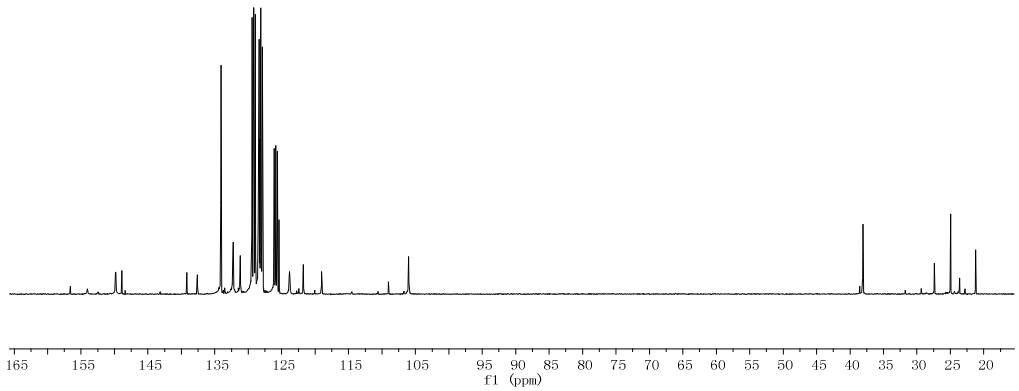

Figure S12. ^{13}C NMR spectrum ([D_5]chlorobenzene, 25 °C) of complex **4**.

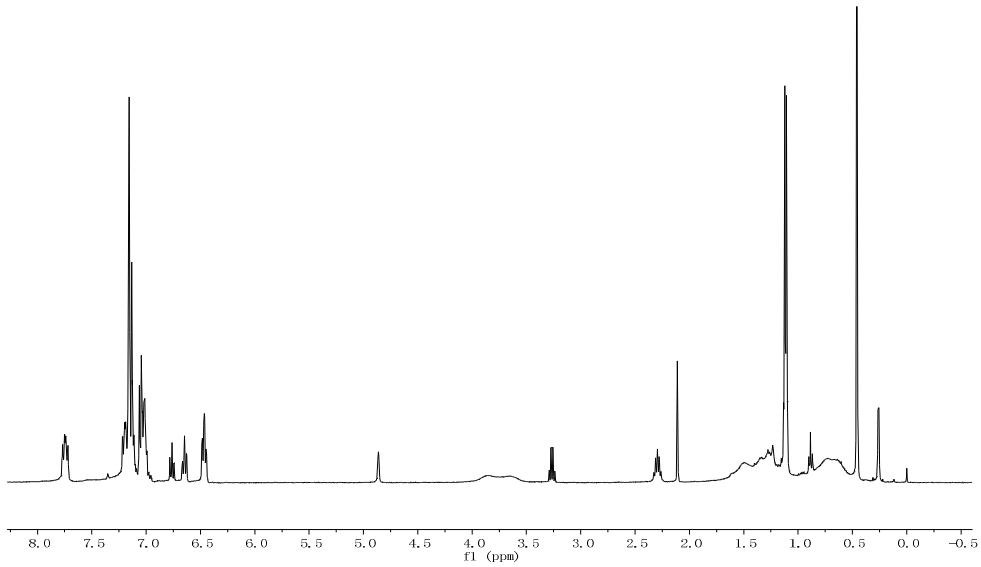

Figure S13. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

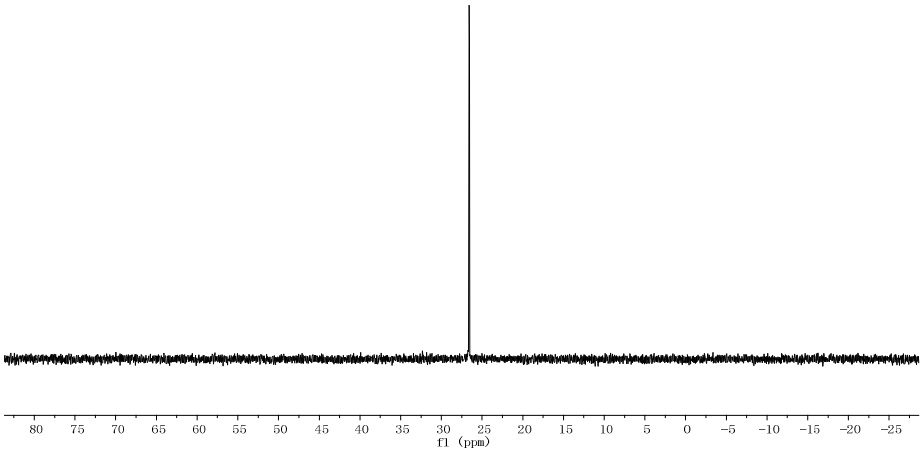

Figure S14. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

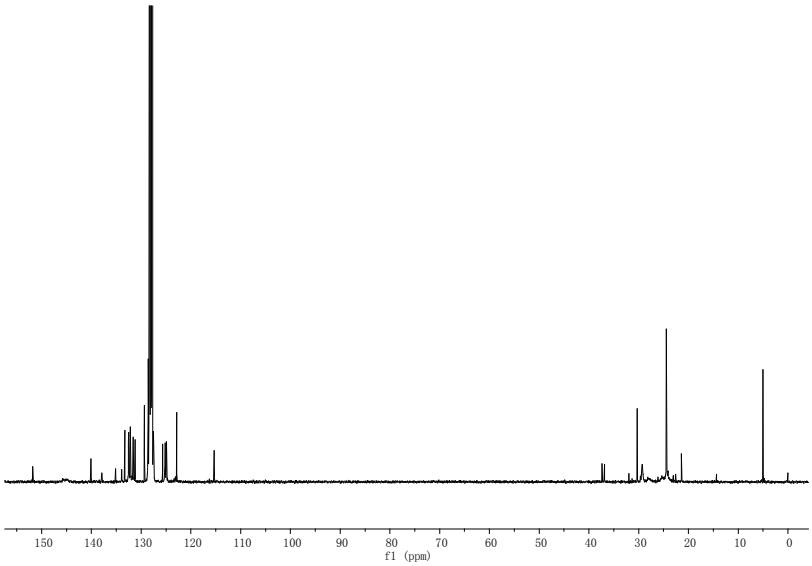

Figure S15. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **9**.

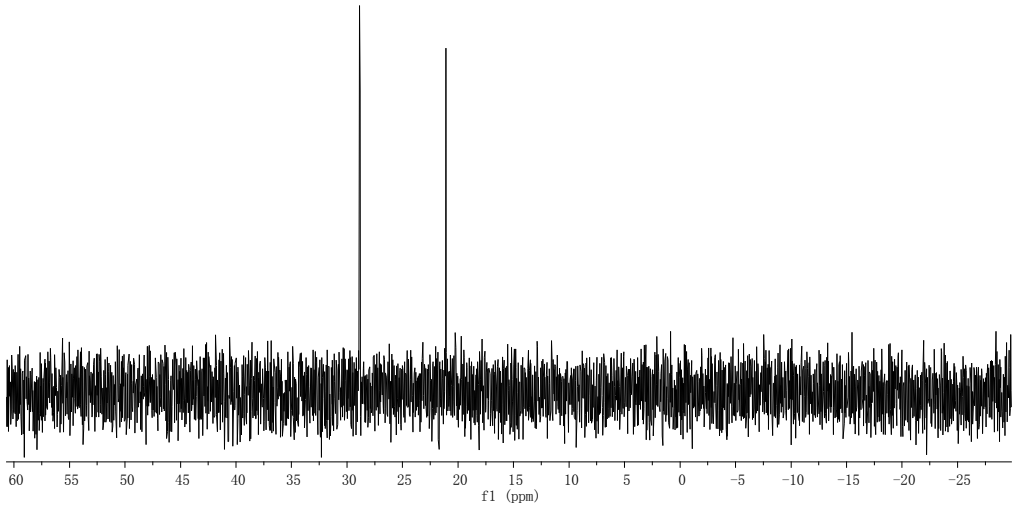

Figure S16. ^{31}P NMR spectrum ([D$_6$]benzene, 25 °C) of complex **9** on heating at 60 ^{o}C for 12h.

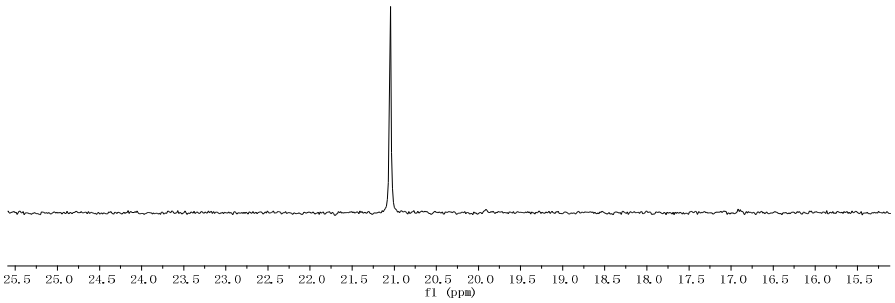

Figure S17. ^{31}P NMR spectrum ([D$_6$]benzene, 25 °C) of ligand HL^2 {HN[Ph$_2$PNC$_6$H$_3$(^{i}Pr)$_2$]$_2$}.

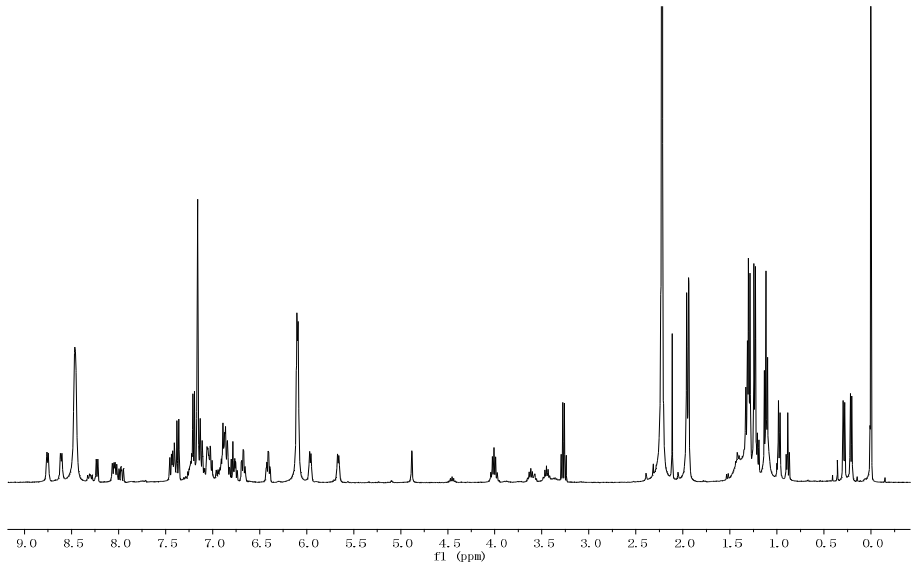

Figure S18. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **9** with 2 equivalent of DMAP at 25 ^{o}C for 12 h.

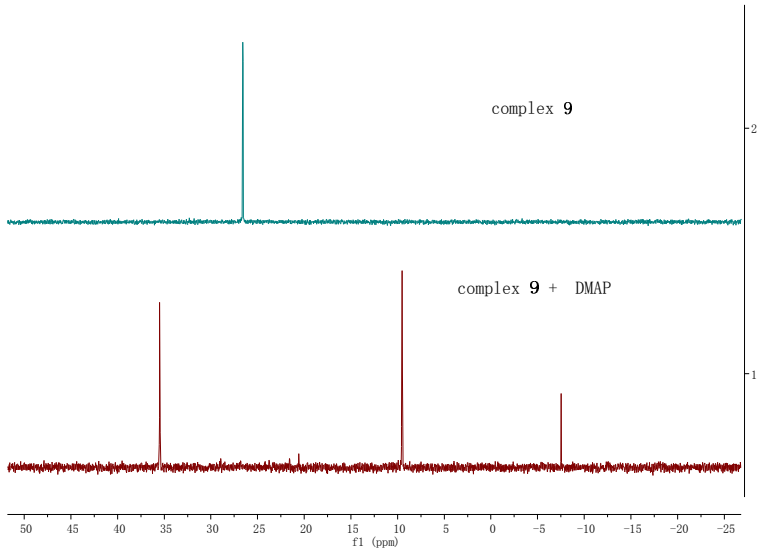

Figure S19. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **9** with 2 equivalent of DMAP at 25 ^{o}C for 12 h.

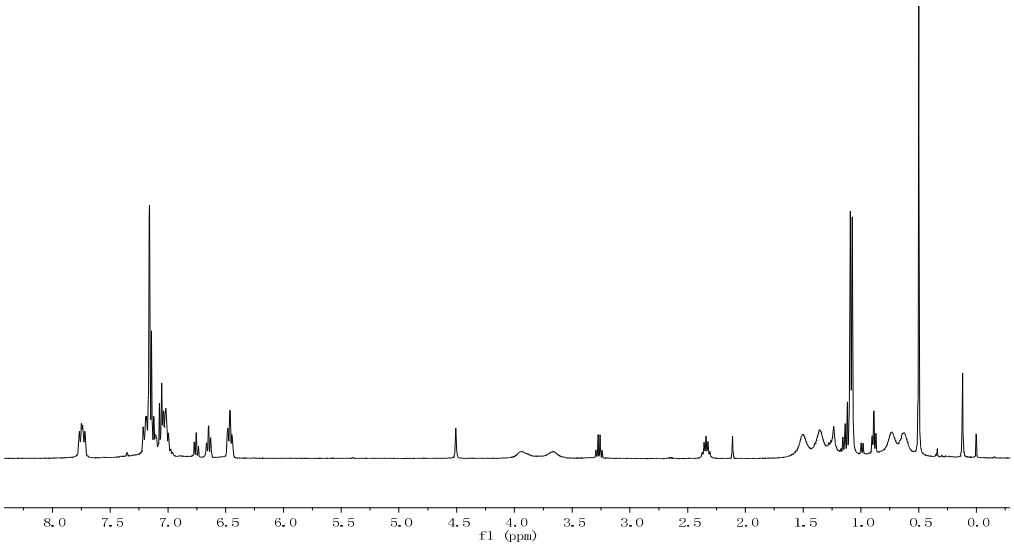

Figure S20. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

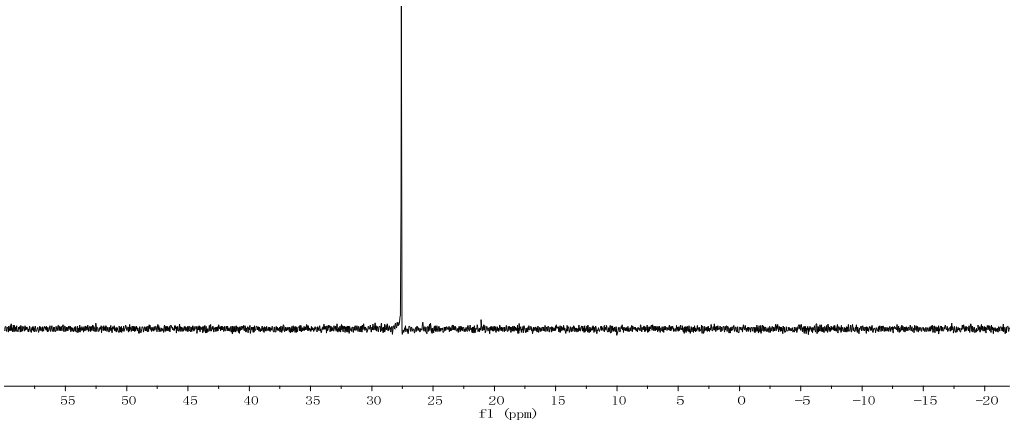

Figure S21. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

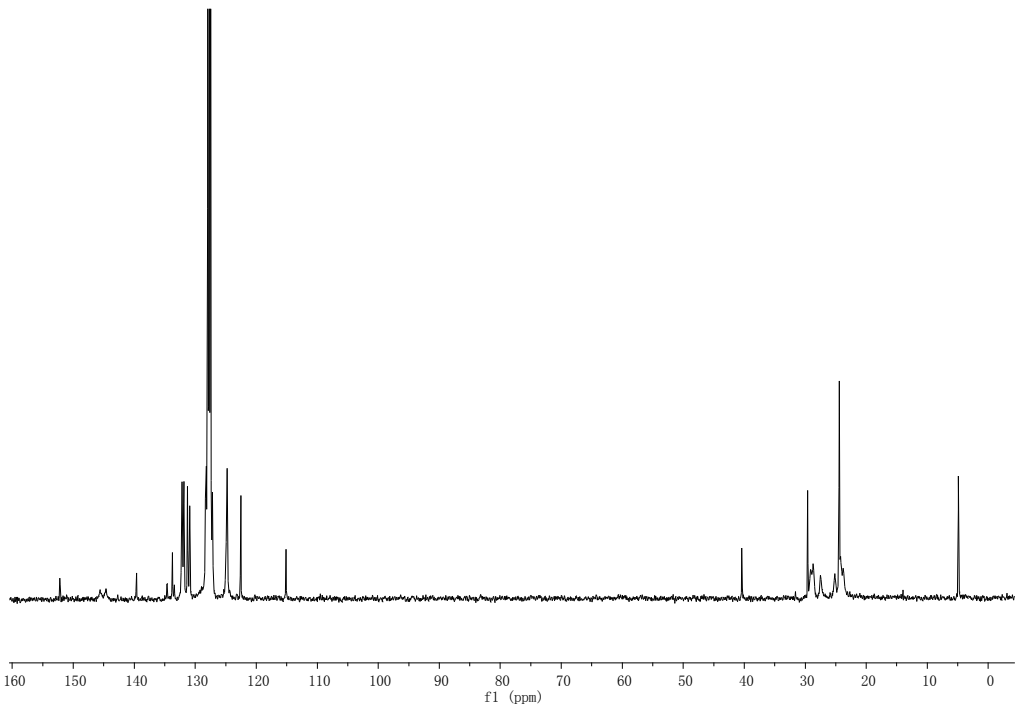

Figure S22. ^{13}C NMR spectrum ([D_6]benzene, 25 °C) of complex **10**.

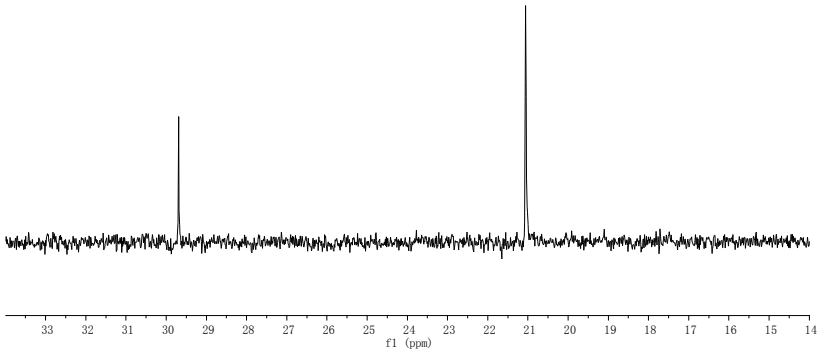

Figure S23. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **10** on heating at 100 ^{o}C for 12h.

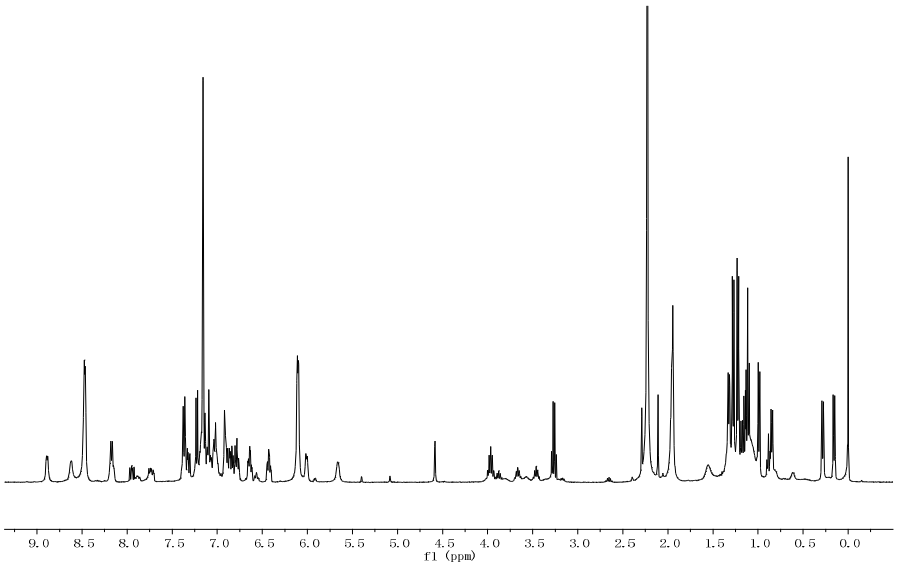

Figure S24. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **10** with 2 equivalent of DMAP at 80 ^{o}C for 5 h.

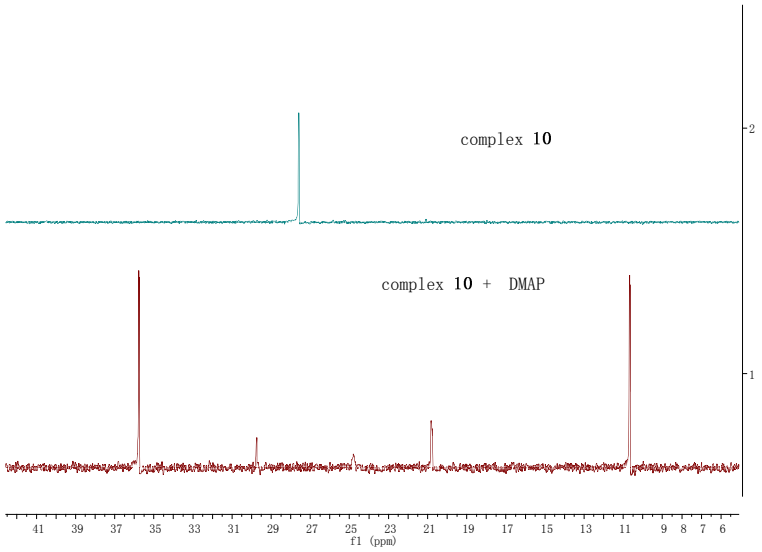

Figure S25. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of reaction of complex **10** with 2 equivalent of DMAP at 80 ^{o}C for 5 h.

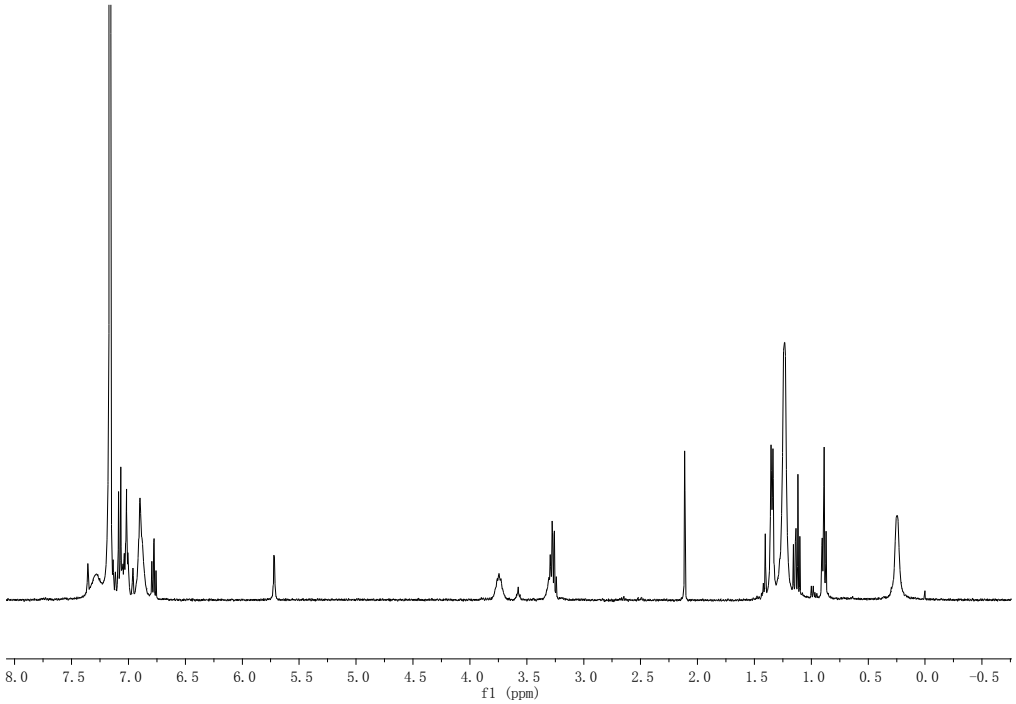

Figure S26. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **11**.

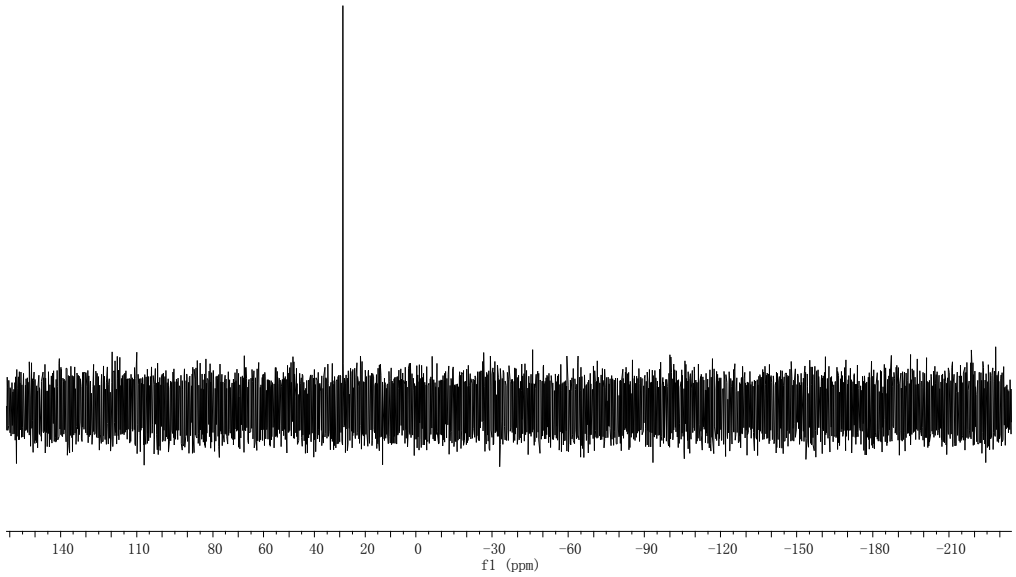

Figure S27. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **11** (very poor solubility).

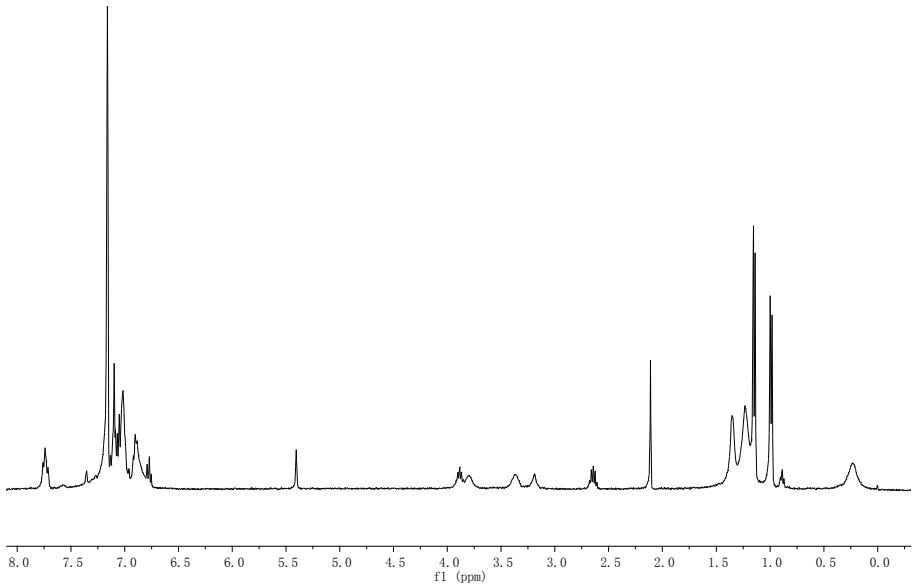

Figure S28. ^{1}H NMR spectrum ([D_6]benzene, 25 °C) of complex **12**.

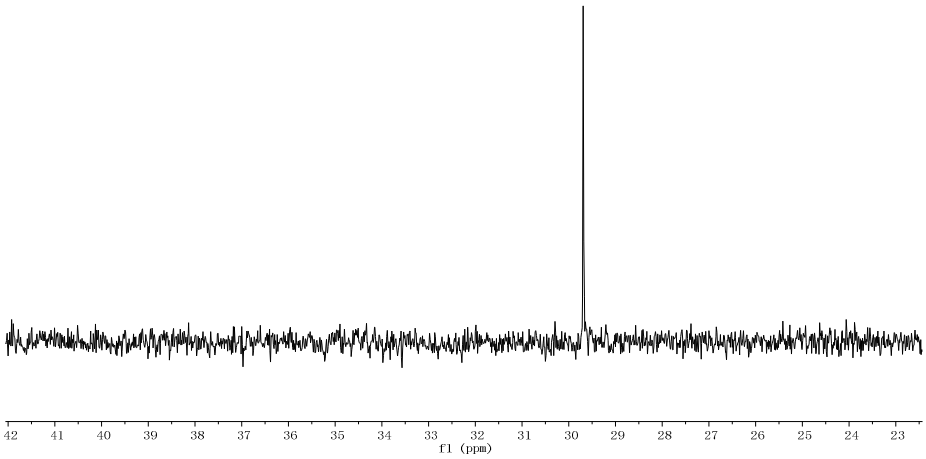

Figure S29. ^{31}P NMR spectrum ([D_6]benzene, 25 °C) of complex **12**.

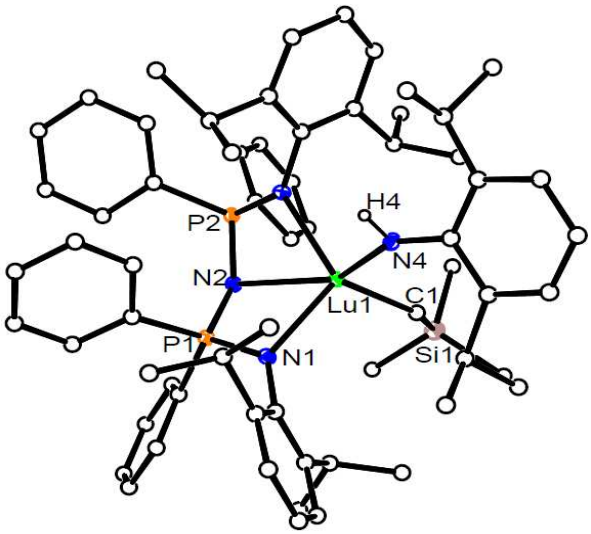

Figure S30. X-ray structure of **10** with 35% probability of thermal ellipsoids.

Hydrogen atoms are partly omitted for clarity.

Selected bond distances (Å) and angles (deg): Lu(1)–N(4) 2.190(4); Lu(1)–N(1) 2.286(3); Lu(1)–N(3) 2.315(4); Lu(1)–C(1) 2.337(5); Lu(1)–N(2) 2.576(4). N(4)–Lu(1)–N(1) 115.85(14); N(4)–Lu(1)–N(3) 93.46(14); N(1)–Lu(1)–N(3) 111.50(13); N(4)–Lu(1)–C(1) 103.65(16); N(1)–Lu(1)–C(1) 108.89(15); N(3)–Lu(1)–C(1) 122.70(15); N(4)–Lu(1)–N(2) 148.17(13); N(1)–Lu(1)–N(2) 62.48(12); N(3)–Lu(1)–N(2) 61.88(12); C(1)–Lu(1)–N(2) 106.65(14).

Table S1. Crystallographic data and structure refinement details for complexes **4, 9, 10** and **11.**

	4 · $2C_7H_8$	**9** · $0.5C_6H_{12}$	**10**	**11** · C_6H_6
formula	$C_{76}H_{83}ScN_8P_2$	$C_{67}H_{88}YN_4P_2Si$	$C_{64}H_{83}LuN_4P_2Si$	$C_{72}H_{90}YN_3P_2$
M_w	1215.40	1128.35	1173.34	1176.34
cryst. system	monoclinic	monoclinic	monoclinic	monoclinic
space group	P2(1)/c	C2/c	Cc	P2(1)/n
a [Å]	13.9704(13)	48.821(3)	23.0407(12)	13.3417(8)
b [Å]	18.0085(17)	14.3262(8)	13.1043(7)	23.5568(13)
c [Å]	26.947(3)	19.1490(12)	21.4908(11)	22.3531(13)

α [°]	90	90	90	90
β [°]	97.053(2)	108.7800(10)	114.0980(10)	94.2320(10)
γ [°]	90	90	90	90
V [Å^3]	6728.2(11)	12680.1(13)	5923.3(5)	7006.1(7)
Z	4	8	4	4
Dcalcd [g cm^{-3}]	1.200	1.182	1.316	1.115
radiation [λ, Å]	$Mo_{K\alpha}$(0.71073)	$Mo_{K\alpha}$(0.71073)	$Mo_{K\alpha}$(0.71073)	$Mo_{K\alpha}$(0.71073)
$2\theta_{max}$ [°]	51.04	50.12	52.08	50.14
μ [mm^{-1}]	0.206	1.031	1.783	0.919
F [000]	2584	4808	2440	2504
no. of obsd reflns	30203	35194	18681	40176
no.of params.refnd	12384	11223	8619	12414
GOF	1.040	0.981	0.987	0.996
R_1 [I>2σ(I)]	0.0688	0.0732	0.0284	0.0573
wR_2 [I>2σ(I)]	0.1936	0.1589	0.0571	0.1263