

Supplementary Materials

Nickel-Catalyzed Ethylene Dimerization Based on PNP(NR₂)₂ Ligands

Chengang Cao, Haonan Fan, Jingyi Zhang, Jing Ma and Tao Jiang *

College of Chemical Engineering and Material Science, Tianjin University of
Science and Technology, Tianjin 300457, China

* Correspondence: jiangtao@tust.edu.cn

Table of Contents

1. Figure S1. - S6. NMR Spectra of complexes **1-3**

2. Table S1. X-ray crystallography of the complexes **1-3**

Figure S1. ^1H NMR Spectrum of complex 1 (CDCl_3)

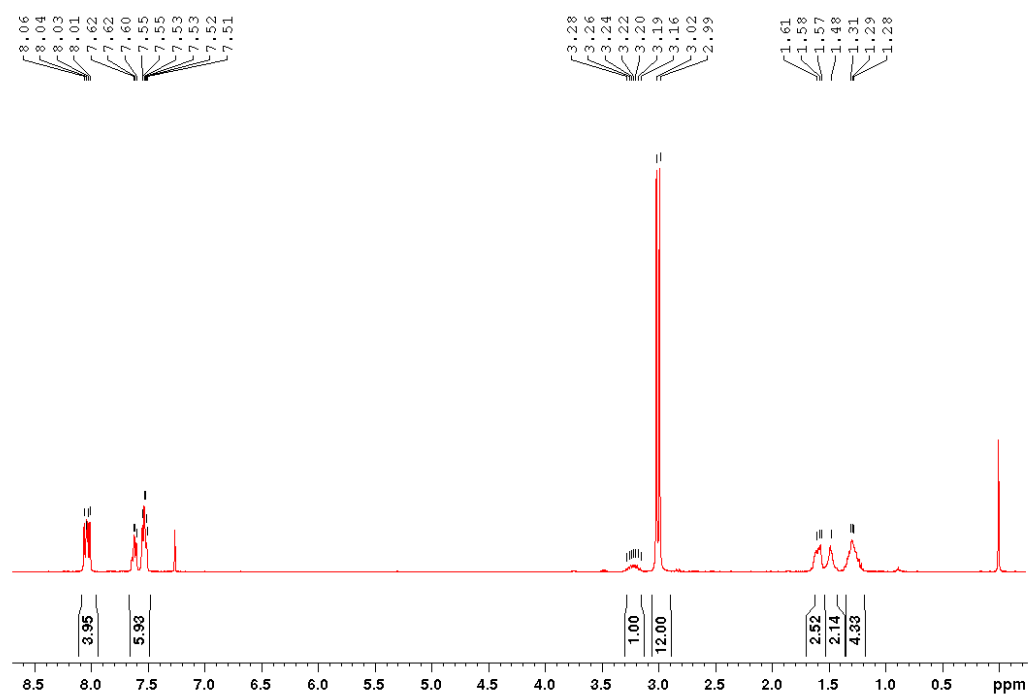


Figure S2. ^{31}P NMR Spectrum of complex 1 (CDCl_3)

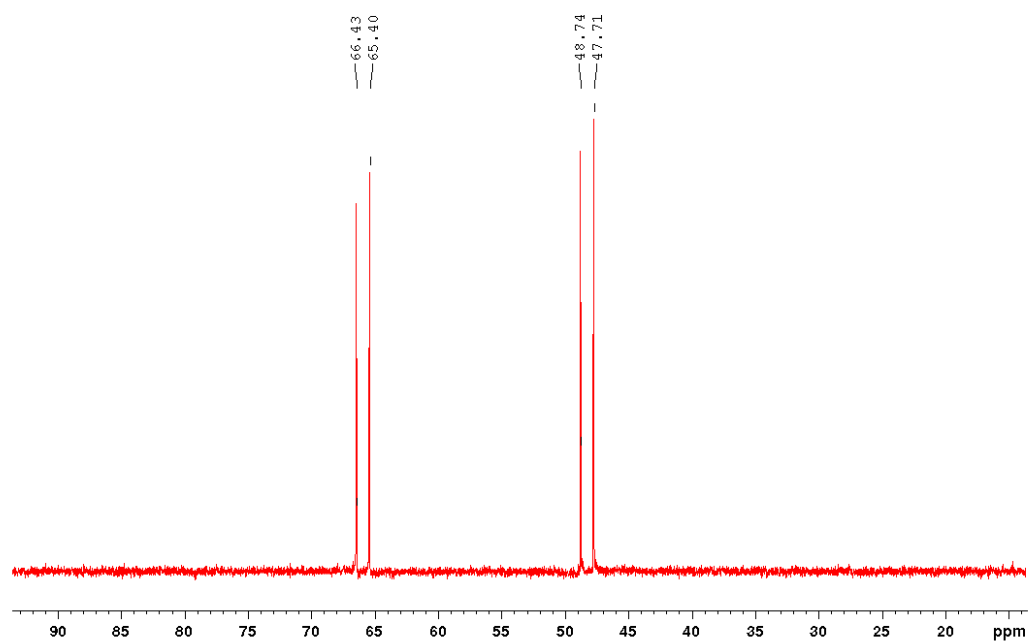


Figure S3. ^1H NMR Spectrum of complex 2 (CDCl_3)

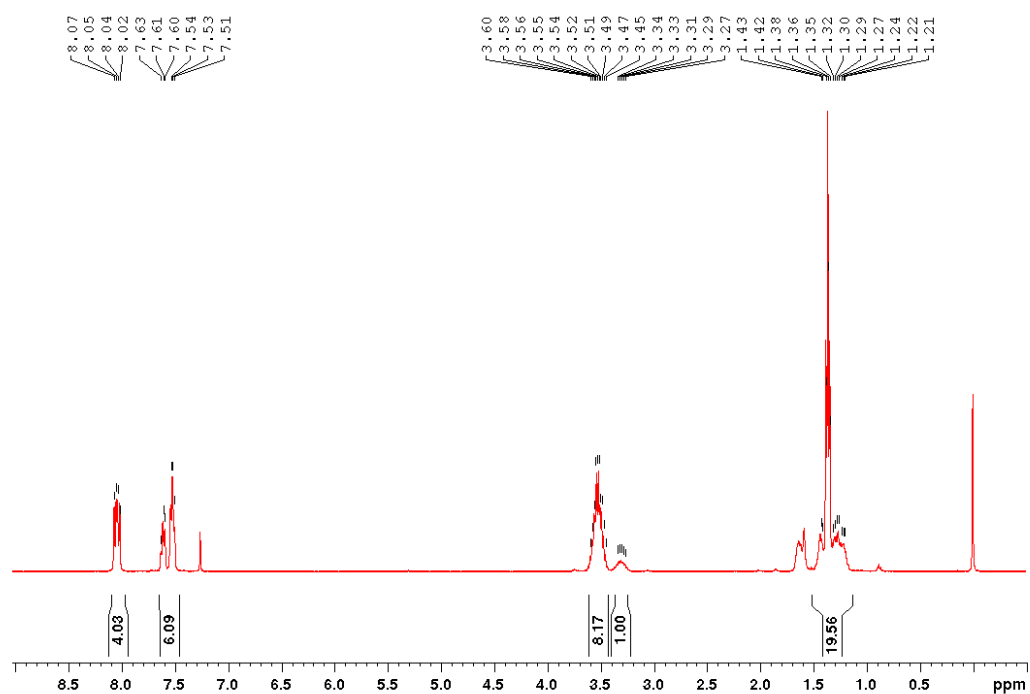


Figure S4. ^{31}P NMR Spectrum of complex 2 (CDCl_3)

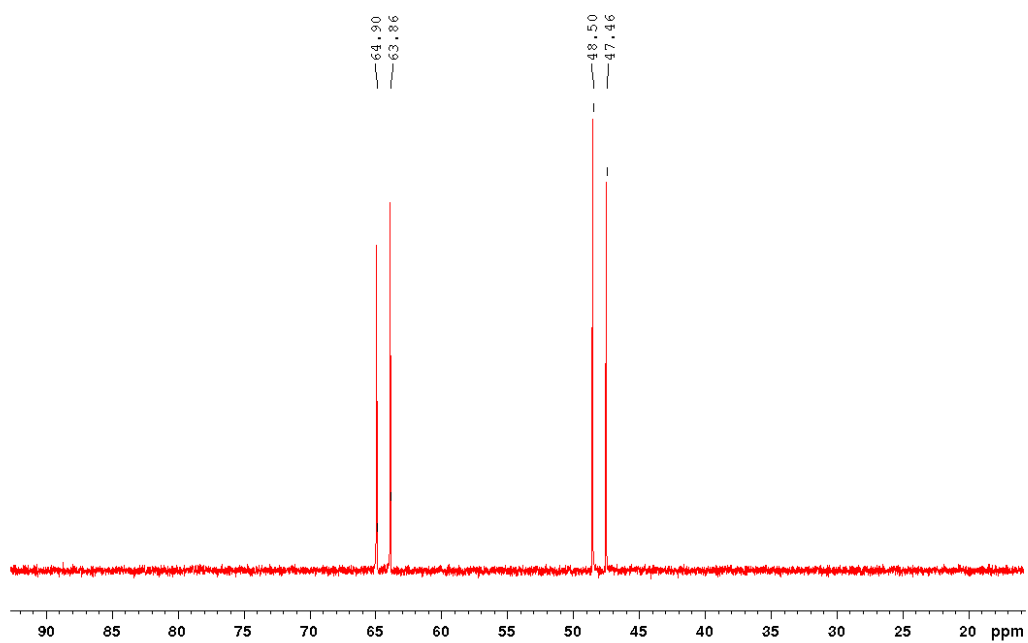


Figure S5. ^1H NMR Spectrum of complex 3 (CDCl_3)

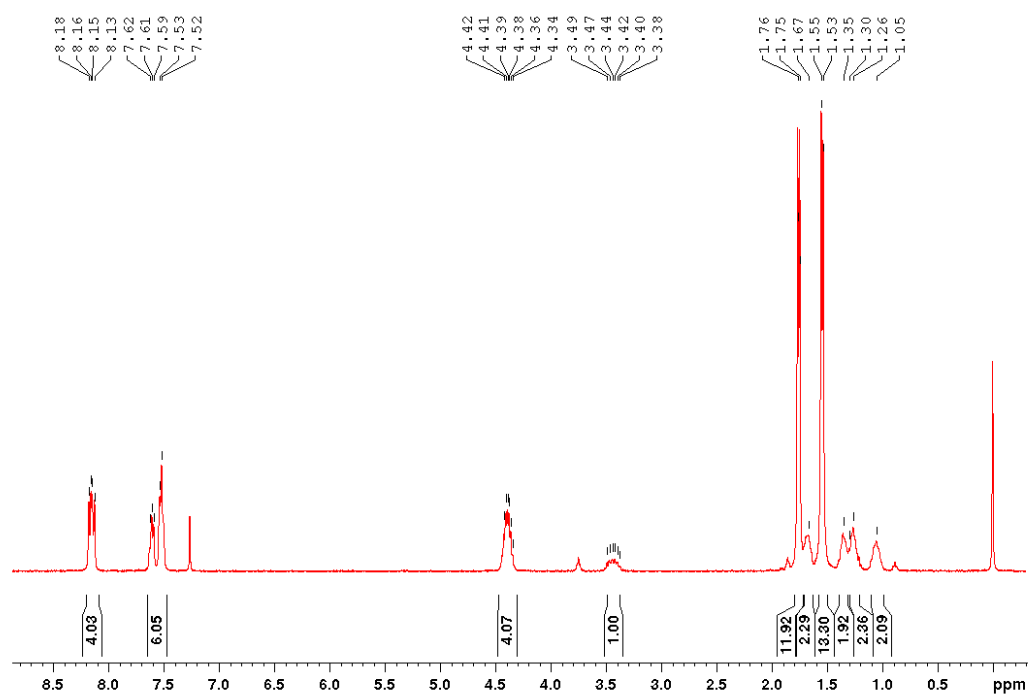


Figure S6. ^{31}P NMR Spectrum of complex 3 (CDCl_3)

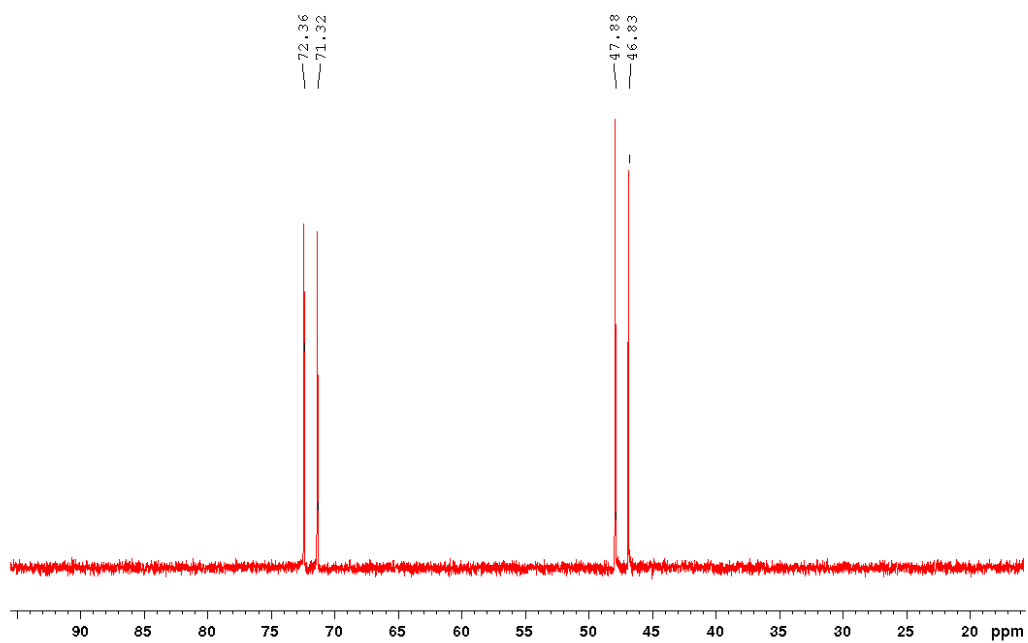


Table S1. Crystallographic Determination Parameters for **1-3** Complexes

Complex	1	2	3
Empirical formula	C ₂₁ H ₃₁ Br ₂ N ₃ NiP ₂	C ₂₅ H ₃₉ Br ₂ N ₃ NiP ₂	C ₂₉ H ₄₇ Br ₂ N ₃ NiP ₂
Formula weight	605.9	662.06	718.16
Temperature	113.15	113.15	113.15
Wavelength	0.71073	0.71073	0.71073
Crystal system, space group	Monoclinic, P2 ₁ /n	Monoclinic, P2 ₁	Monoclinic, P2 ₁
Unit cell dimensions	a = 9.4766(3) Å; α = 90° b = 14.7740(4) Å; β = 96.766(3)° c = 17.6542(6) Å; γ = 90°	a = 9.3488(4) Å; α = 90° b = 15.3605(6) Å; β = 103.789(4)° c = 10.1924(4) Å; γ = 90°	a = 10.1526(5) Å; α = 90° b = 15.9976(9) Å; β = 94.360(4)° c = 19.0343(8) Å; γ = 90°
Volume	2454.50(13)	1421.47(10)	3082.6(3)
Z, Calculated density	4, 1.640 g·cm ⁻³	2, 1.547 g·cm ⁻³	4, 1.547 g·cm ⁻³
Absorption coefficient	4.190	3.625	3.349
F(000)	1224.0	676.0	1480.0
Theta range for data collection	4.646 to 65.878°	4.114 to 65.76°	4.024 to 56.564°
Limiting indices	-13 ≤ h ≤ 13 -21 ≤ k ≤ 21 -25 ≤ l ≤ 26	-13 ≤ h ≤ 14 -20 ≤ k ≤ 22 -15 ≤ l ≤ 15	-13 ≤ h ≤ 13 -21 ≤ k ≤ 20 -24 ≤ l ≤ 25
Reflections collected/unique	30638/8544[R(int)=0.0563]	18043/8291[R(int)=0.0509]	31127/7651[R(int)=0.0825]
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data/restraints/parameters	8544/250/313	8291/1/303	7651/0/343
Goodness-of-fit on F ²	1.024	1.002	1.013
Final R indices [I > 2sigma(I)]	R ₁ = 0.0460, wR ₂ = 0.0920	R ₁ = 0.0433, wR ₂ = 0.0791	R ₁ = 0.0454, wR ₂ = 0.0778
R indices (all data)	R ₁ = 0.0767, wR ₂ = 0.1049	R ₁ = 0.0617, wR ₂ = 0.0880	R ₁ = 0.0844, wR ₂ = 0.0894