

Supporting Information for:
Synthesis and Application of Binuclear α -Diimine Nickel/Palladium
Catalysts with Conjugated Backbone

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Table S1. Crystallographic data for complex**C5**

data	C5
Empirical formula	C ₆₆ H ₈₂ Cl ₆ N ₄ Pd ₂
Formula Wt	1356.86
Temp.(K)	120(2)
Crystsyst	orthorhombic
Space group	P b c a
a(Å)	19.3028(6)
b(Å)	14.8149(4)
c(Å)	23.5131(5)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V(Å ³)	6724.0(3)
Z	4
D _t (Mg/m ³)	1.340
Abs coeff (mm ⁻¹)	0.814
F(000)	2800
Crystal size (mm)	0.46 × 0.42 × 0.38
θ range (deg)	2.88 to 25.500
Index ranges	-18= h ≤23, -17= k ≤17, -28= l ≤23

No. of reflns collected	28239
No. of indepreflns	6248
Completeness to $\theta=25.5$	0.998
Absorption correction	multi-scan
Max. and min. transmission	0.7474 and 0.7060
Refinement method	None
No. of data / restraints / params	6248/420/129 1.033
Goodness-of-fit on F^2	R1 = 0.0472,
Final R indices [$I>2\sigma(I)$]	wR2 = 0.1124
	R1 = 0.1296,
R indices(all data)	wR2 = 0.1296

Table S2. Selected bond lengths (Å) and angles (deg) for **C5**

Bond lengths(Å)		Bond Angles(°)	
Pd(1)-N(1)	2.085(3)	N(2)-C(1)-C(2)	119.1 (4)
Pd(1)-N(2)	2.136(2)	N(2)-C(1)-C(6)	117.9(4)
Pd(1)-Cl(1)	2.256(2)	Cl(1)-Pd(1)-N(2)	99.9(1)
Pd(1)-C(1)	2.035(20)	C(1)-Pd(1)-N(1)	92.5.7(5)
N(1)-C(18)	1.277(5)	Pd(1)-N(2)-C(13)	111.9(3)
N(1)-C(20)	1.440(5)	Pd(1)-N(1)-C(18)	113.2(3)
N(2)-C(1)	1.434(5)	N(1)-C(20)-C(25)	118.9(4)
N(2)-C(13)	1.283(5)	N(2)-C(20)-C(21)	117.7(4)

Table S3. Crystallographic data for complex**CP**

data	CP
Empirical formula	C ₂₁ H ₂₂ Br ₂ N ₄ Ni
Formula Wt	619.86
Temp.(K)	120(2)
Crystalsyst	hexagonal
Space group	P 61 2
a(Å)	9.1161(2)
b(Å)	9.1161(2)
c(Å)	50.8316(9)
α (deg)	90.00
β (deg)	90.00
γ (deg)	120.00
V(Å ³)	3658.32(9)
Z	6
D _t (Mg/m ³)	1.688
Abs coeff (mm ⁻¹)	7.124
F(000)	1848.0
Crystal size (mm)	0.28 × 0.26 × 0.22

θ range (deg)	2.88 to 67.43
Index ranges	-10= h <= 9, -10= k <= 10, -59= l <= 57
No. of reflns collected	13059
No. of indepreflns	2183
Completeness to θ =67.43	1.51
Absorption correction	multi-scan
Max. and min. transmission	0.240 and 0.303
Refinement method	None
No. of data / restraints / params	2183/140/140 1.028
Goodness-of-fit on F^2	$R_1 = 0.0228$,
Final R indices [$I > 2\sigma(I)$]	$wR_2 = 0.0767$ $R_1 = 0.0293$,
R indices(all data)	$wR_2 = 0.0767$

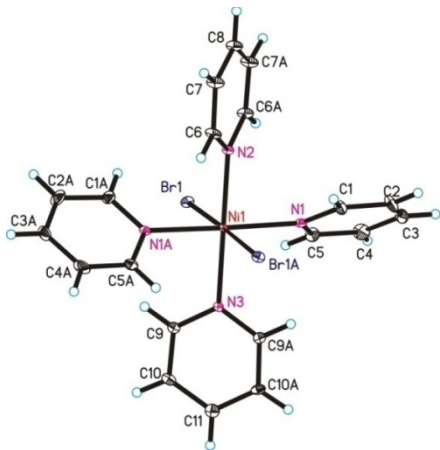


Figure S1. ORTEPdiagram of **CP**.Hydrogen atoms have been omitted for clarity.

Table S4. Selected bond lengths (Å) and angles (deg) for **CP**

Bond lengths(Å)			Bond Angles(°)
N(1)-Ni(1)	2.154(3)	N(1)-Ni(1)-N(2)	89.24 (8)
N(2)-Ni(1)	2.094(4)	N(1)-Ni(1)-N(3)	90.76(8)
N(3)-Ni(1)	2.121(4)	N(1)-Ni(1)-Br(1)	89.15(8)
N(1A)-Ni(1)	2.035(20)	N(1)-Ni(1)-Br(1A)	90.88(8)
Br(1)-Ni(1)	2.625(0)	N(1A)-Ni(1)-N(2)	89.24(8)
Br(1A)-Ni(1)	2.625(0)	N(1A)-Ni(1)-N(3)	90.79(8)
N(1)-C(1)	1.348(5)	N(1A)-Ni(1)-Br(1)	90.88(8)
N(1)-C(5)	1.342(5)	N(1A)-Ni(1)-Br(1A)	89.15(4)

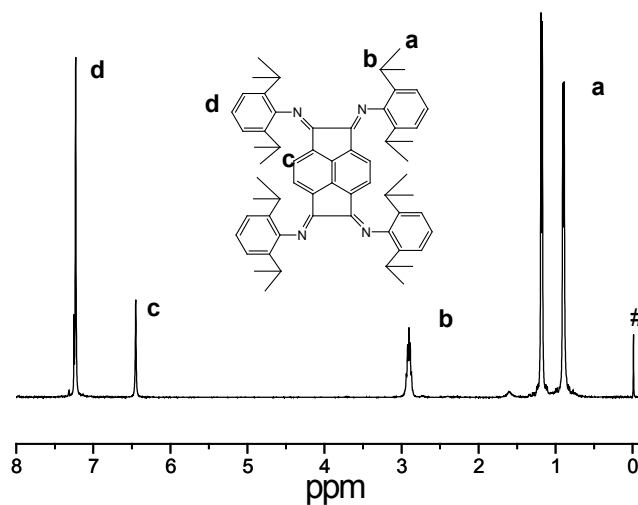


Figure S2. ^1H -NMR of compound **L2** in CDCl_3 (#, TMS).

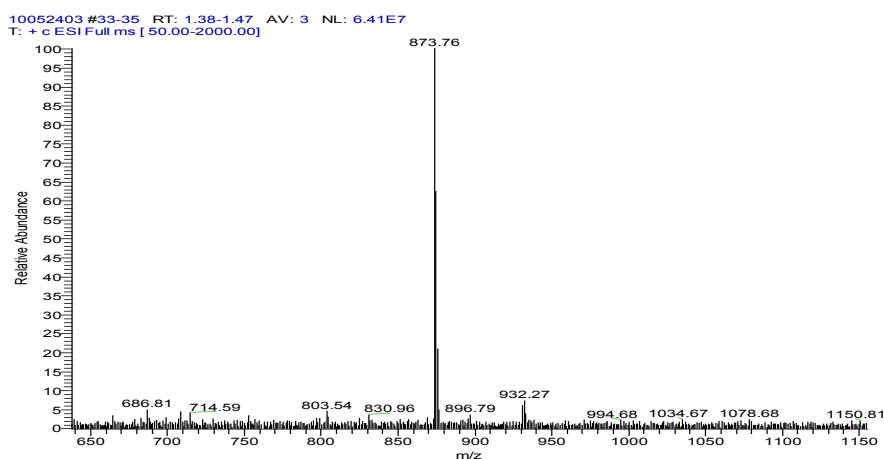


Figure S3. ESI-MS of compound **L2**.

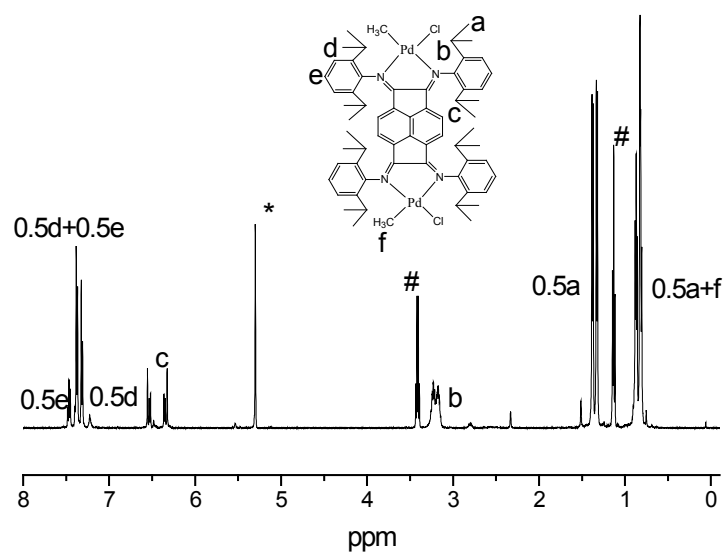


Figure S4. ^1H -NMR of catalyst **C5** in CD_2Cl_2 (#, $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$; *, CH_2Cl_2).

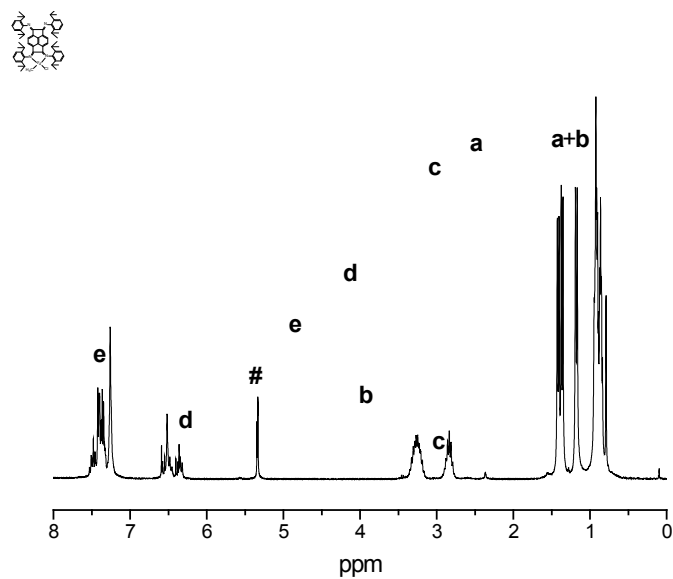


Figure S5. ^1H -NMR of catalyst **C3** in CD_2Cl_2 (#, CH_2Cl_2).

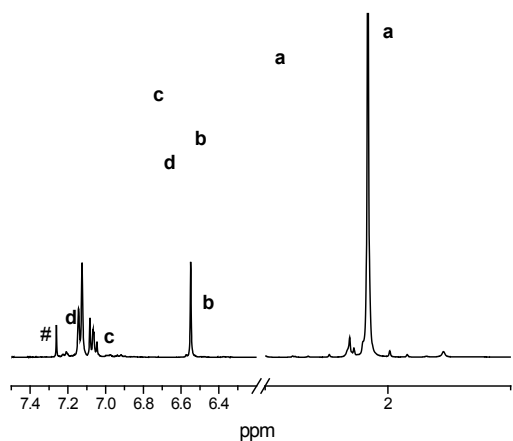


Figure S6. ¹H-NMR of compound **L1** in CDCl₃ (#, CHCl₃).

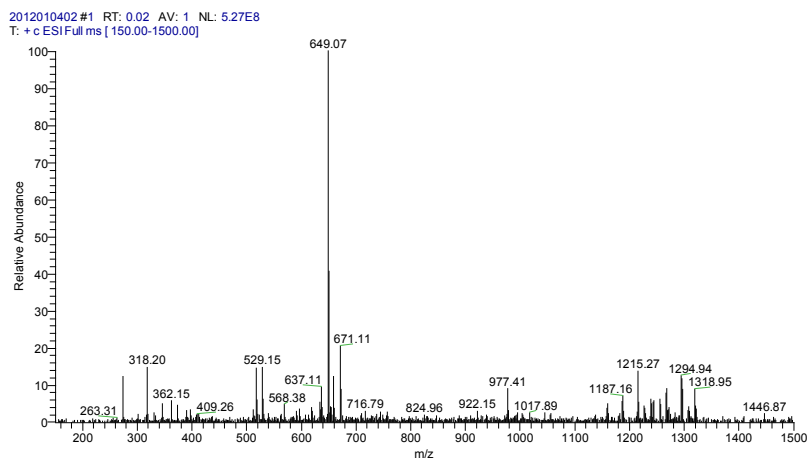


Figure S7. ESI-MS of compound **L1**.

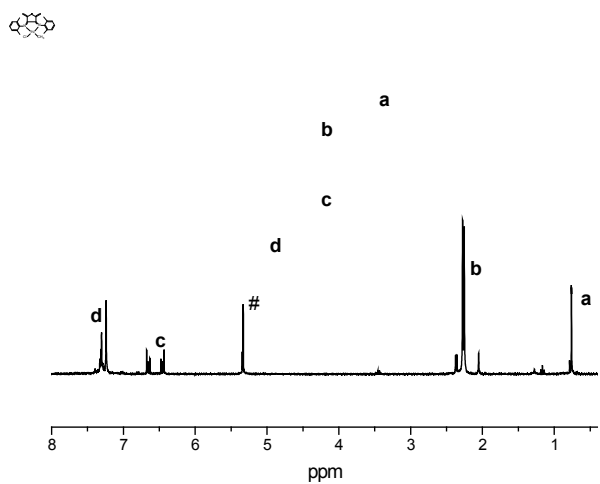


Figure S8. ¹H-NMR of catalyst **C4** in CD₂Cl₂ (#, CH₂Cl₂).

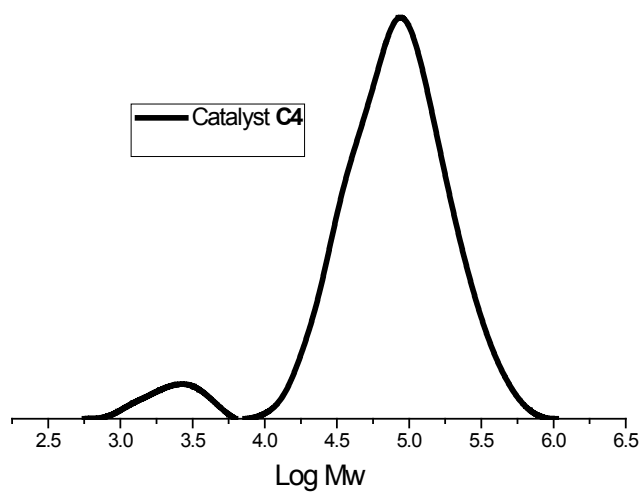


Figure S8.GPC curves of polyethylene prepared by catalyst **C4** with 2 equiv. of **Li**.