

Supplementary Materials: Geometry Constrained *N*-(5,6,7-Trihydroquinolin-8-ylidene)arylamino palladium Dichlorides Complexes: Catalytic Behavior toward MA, MA-*co*-NB Polymerization and Heck Coupling

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Table S1. Selected bond lengths (Å) and angles (°) for complexes Pd4 and Pd5.

Pd4		Pd5	
Bond lengths (Å)			
Pd(1)-N(2)	2.0209(17)	Pd(1)-N(2)	2.0354(17)
Pd(1)-N(1)	2.0254(18)	Pd(1)-N(1)	2.0253(18)
Pd(1)-Cl(2)	2.2734(11)	Pd(1)-Cl(2)	2.2973(8)
Pd(1)-Cl(1)	2.2983(9)	Pd(1)-Cl(1)	2.2728(11)
N(1)-C(1)	1.330(2)	N(1)-C(1)	1.331(3)
C(7)-C(8)	1.494(3)	C(7)-C(8)	1.497(3)
Bond angles (°)			
N(2)-Pd(1)-N(1)	80.31(7)	N(2)-Pd(1)-N(1)	80.37(7)
N(2)-Pd(1)-Cl(2)	94.26(5)	N(1)-Pd(1)-Cl(1)	174.96(5)
N(1)-Pd(1)-Cl(2)	172.03(5)	N(2)-Pd(1)-Cl(1)	94.63(6)
N(2)-Pd(1)-Cl(1)	171.81(5)	N(1)-Pd(1)-Cl(2)	94.28(6)
N(1)-Pd(1)-Cl(1)	95.33(6)	N(2)-Pd(1)-Cl(2)	174.05(5)
Cl(2)-Pd(1)-Cl(1)	90.75(3)	Cl(1)-Pd(1)-Cl(2)	90.69(4)
C(1)-N(1)-C(9)	119.13(17)	C(1)-N(1)-C(9)	119.16(17)
C(1)-N(1)-Pd(1)	127.64(14)	C(1)-N(1)-Pd(1)	127.93(15)
C(9)-N(1)-Pd(1)	113.19(13)	C(9)-N(1)-Pd(1)	112.90(13)
C(8)-N(2)-C(10)	120.44(16)	C(8)-N(2)-C(10)	121.19(17)
C(8)-N(2)-Pd(1)	115.48(13)	C(8)-N(2)-Pd(1)	114.78(13)
C(10)-N(2)-Pd(1)	123.76(12)	C(10)-N(2)-Pd(1)	124.03(13)

Table S2. Crystal data and structure refinement for complexes **Pd4** and **Pd5**.

	Pd4	Pd5
Crystal color	Yellow	Yellow
Empirical formula	C ₁₈ H ₂₀ Cl ₂ N ₂ Pd	C ₂₀ H ₂₄ Cl ₂ N ₂ Pd
Formula weight	441.66	469.73
Temperature/K	173 (2)	173 (2)
Wavelength/Å	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P21/a	P-1
<i>a</i> /Å	7.4548(15)	8.3628(17)
<i>b</i> /Å	30.651(6)	8.5040(17)
<i>c</i> /Å	8.2911(17)	15.861(3)
Beta/°	112.43(3)	74.93(3)
Volume/Å ³	1751.2(6)	966.4(3)
<i>Z</i>	4	2
<i>D</i> _{calcd} /(g·cm ⁻³)	1.675	1.614
μ /mm ⁻¹	1.365	1.242
<i>F</i> (000)	888	476
Crystal size/mm	0.39 × 0.27 × 0.07	0.46 × 0.20 × 0.11
θ range (°)	2.66–27.49	2.79–24.99
	−9 ≤ <i>h</i> ≤ 9	−9 ≤ <i>h</i> ≤ 9
Limiting indices	−39 ≤ <i>k</i> ≤ 39	−10 ≤ <i>k</i> ≤ 10
	−10 ≤ <i>l</i> ≤ 10	−18 ≤ <i>l</i> ≤ 18
No. of rflns collected	18,759	10,319
No. unique rflns	3989	3351
R(int)	0.0296	0.0234
No. of params	211	229
Completeness to θ	99.1%	98.9%
Goodness of fit on <i>F</i> ²	0.986	1.039
Final <i>R</i> indices [<i>I</i> > 2 Σ (<i>I</i>)]	<i>R</i> 1 = 0.0278 <i>wR</i> 2 = 0.0726	<i>R</i> 1 = 0.0197 <i>wR</i> 2 = 0.1208
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0283 <i>wR</i> 2 = 0.0732	<i>R</i> 1 = 0.0201 <i>wR</i> 2 = 0.0555
Largest diff. peak, and hole/(e·Å ⁻³)	1.206 and −0.706	0.379 and −0.458