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Supporting Information

Dinuclear NHC–Palladium Complexes Containing Phosphine Spacers: Synthesis, X-Ray Structures and Their Catalytic Activities towards Hiyama Coupling Reaction

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Table S1 Selected bond lengths [Å] and angles [deg] for compounds **1–6**

	1 •2CH ₂ Cl ₂	2 •2CH ₂ Cl ₂			3	4			5	6 •H ₂ O
Pd(1)–C(1)	2.043(5)	2.032(10)	Pd(2)–C(41)	2.036(9)	2.031(6)	2.047(5)	Pd(2)–C(28)	2.041(5)	1.992(11)	2.038(3)
Pd(1)–Cl(1)	2.3055(12)	2.289(3)	Pd(2)–Cl(3)	2.274(3)	2.285(2)	2.2985(15)	Pd(2)–Cl(3)	2.2879(15)	2.280(4)	2.2790(8)
Pd(1)–Cl(2)	2.2857(14)	2.309(3)	Pd(2)–Cl(4)	2.294(3)	2.255(2)	2.2791(15)	Pd(2)–Cl(4)	2.3003(14)	2.193(4)	2.2818(8)
Pd(1)–P(1)	2.3177(12)	2.288(3)	Pd(2)–P(2)	2.307(3)	2.317(2)	2.3107(15)	Pd(2)–P(2)	2.3067(15)	2.278(3)	2.3004(8)
C(1)–Pd(1)–Cl(1)	91.15(15)	91.8(3)	C(41)–Pd(2)–Cl(3)	90.7(3)	89.06(17)	89.63(14)	C(28)–Pd(2)–Cl(3)	90.85(14)	90.8(4)	92.06(8)
C(1)–Pd(1)–Cl(2)	89.51(15)	88.0(3)	C(41)–Pd(2)–Cl(4)	89.2(3)	90.33(17)	91.30(14)	C(28)–Pd(2)–Cl(4)	89.69(14)	88.6(4)	88.53(8)
Cl(1)–Pd(1)–P(1)	85.73(4)	92.40(11)	Cl(3)–Pd(2)–P(2)	92.53(11)	87.56(7)	87.14(5)	Cl(3)–Pd(2)–P(2)	92.21(6)	86.63(12)	88.36(3)
Cl(2)–Pd(1)–P(1)	93.83(5)	88.28(11)	Cl(4)–Pd(2)–P(2)	88.13(11)	93.41(7)	91.86(6)	Cl(4)–Pd(2)–P(2)	87.28(5)	94.33(13)	91.31(3)
PdCPCl ₂ /carbene dihedral angle	69.53	77.33		77.50	82.55	68.69		78.51	76.96	59.73
carbene/Pd1P1P1A Pd1A ^a dihedral angle	38.84 ⁱ	70.12 ⁱⁱ		69.93 ⁱⁱ	30.89 ⁱⁱⁱ		Pd1P1P2Pd2 torsion angle	44.34	14.62 ^{iv}	89.96 ^v
PdCPCl ₂ /Pd1P1P1A Pd1A dihedral angle	72.16 ⁱ	33.52 ⁱⁱ		33.57 ⁱⁱ	67.23 ⁱⁱⁱ				62.84 ^{iv}	30.46 ^v

^a Symmetry codes: ⁱ1 – x, 1 – y, 1 – z; ⁱⁱ2 – x, 1 – y, –z; ⁱⁱⁱ1 – x, –y, –z; ^{iv}–x, –y, 1 – z; ^v–x, 2 – y,

^1H NMR, ^{13}C NMR and ^{31}P NMR spectra















