

**Application Guide for Palladium
Catalyzed Cross-Coupling Reactions**

Add Aldrich



Common Cross-Coupling Reactions

Negishi (C-C)



R¹ = alkenyl, (hetero)aryl, alkynyl, acyl
 R² = alkenyl, (hetero)aryl, alkynyl, alkyl
 X = Cl, Br, I, OTf, OAc

Heck (C-C)



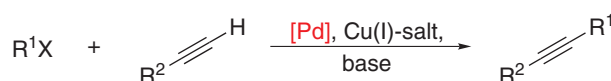
R¹ = alkenyl, (hetero)aryl, alkyl (w/o β-hydrogens)
 R² = alkenyl, (hetero)aryl, alkyl
 X = Cl, Br, I, OTf, OTs, N₂⁺

Suzuki (C-C)



R¹ = alkenyl, (hetero)aryl, alkyl
 R² = alkenyl, (hetero)aryl, alkynyl, alkyl
 Y = alkyl, OH, O-alkyl
 X = Cl, Br, I, OTf

Sonogashira (C-C)



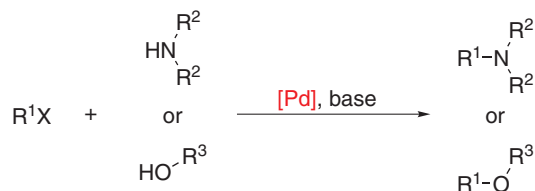
R¹ = alkenyl, (hetero)aryl
 R² = H, alkenyl, (hetero)aryl, alkyl, SiR₃
 X = Cl, Br, I, OTf

Stille (C-C)



R¹ = alkenyl, (hetero)aryl, acyl
 R² = alkenyl, (hetero)aryl, alkyl
 X = Cl, Br, I, OTf

Buchwald-Hartwig (C-N and/or C-O)





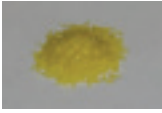

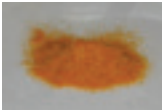


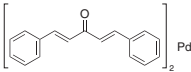

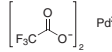

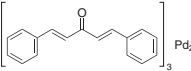
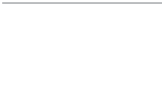
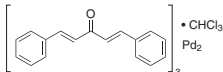

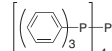

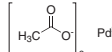


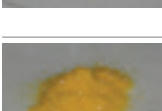
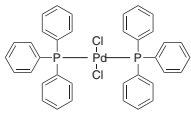
R¹ = (hetero)aryl
 R² = 1° or 2° aryl or alkyl
 R³ = 1°, 2°, or 3° alkyl, aryl
 X = Cl, Br, I, OTf

References:


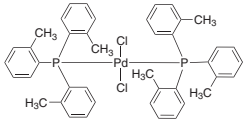
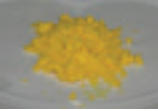
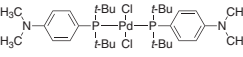



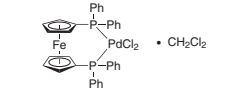

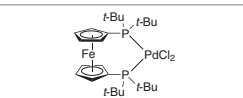

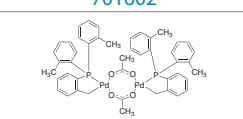

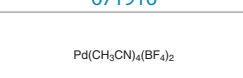

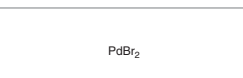


- Negishi, E., *Handbook of Organopalladium Chemistry for Organic Synthesis*; John Wiley & Sons: New York, NY, 2002.
- Tsuji, J., *Palladium Reagents and Catalysts: New Perspectives for the 21st Century*; John Wiley & Sons: Chichester, West Sussex, England, 2004.
- Kürti, L. and Czakov, B. *Strategic Applications of Named Reactions in Organic Synthesis*; Elsevier Academic Press: Burlington, MA, 2005.
- Li, J. J. *Named Reactions for Homologations*; John Wiley & Sons: Hoboken, NJ, 2009.

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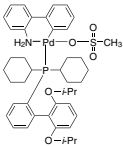

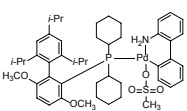

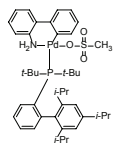

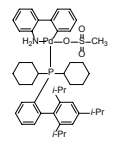

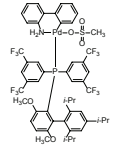

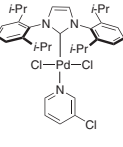
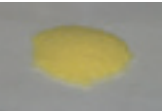
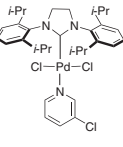

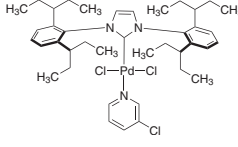
Palladium Catalysts and Precursors

Structure and Cat. No.	Common Name	CAS No.	Mol. Wt.	Color	Stability	Negishi	Suzuki	Stille	Heck	Sonogashira	Buchwald-Hartwig
  209015	Pd(acac) ₂	14024-61-4	304.64	Yellow	Air Stable		X		X		X
  222380	[Pd(allyl)Cl] ₂	12012-95-2	365.89	Yellow	Air/ Moisture Sensitive		X	X	X	X	
  225657	Pd(MeCN) ₂ Cl ₂	14592-56-4	259.43	Dark Orange	Air Stable	X	X	X		X	
  227994	Pd(dba) ₂	32005-36-0	575.00	Black	Air/Mois- ture Sensitive	X	X	X	X		X
  299685	Pd(TFA) ₂	42196-31-6	332.45	Brown	Air Stable		X		X	X	X
  328774	Pd ₂ (dba) ₃	51364-51-3	915.72	Dark Purple to Black	Air Stable	X	X		X		X
  366315 (chloroform adduct of 328774)	Pd ₂ (dba) ₃ · CHCl ₃	52522-40-4	1035.10	Purple	Air Stable		X		X		X
  216666 697265	Pd(PPh ₃) ₄	14221-01-3	1155.56	Canary Yellow	Air/ Moisture Sensitive	X	X	X		X	X
  520764	Pd(OAc) ₂	3375-31-3	224.51	Orange- Brown	Air Stable	X	X	X	X		X
  403237	Pd(PCy ₃) ₂ Cl ₂	29934-17-6	738.18	Yellow	Air Stable		X		X	X	X
  412740	Pd(PPh ₃) ₂ Cl ₂	13965-03-2	701.90	Yellow	Air/Mois- ture Sensitive	X	X	X	X	X	

Application Guide for Palladium Catalyzed Cross-Coupling Reactions

Structure and Cat. No.	Common Name	CAS No.	Mol. Wt.	Color	Stability	Negishi	Suzuki	Stille	Heck	Sonogashira	Buchwald-Hartwig
  453048	Pd[P(o-tol) ₃] ₂ Cl ₂	40691-33-6	786.06	Yellow	Air/Moisture Sensitive	X	X	X	X		X
  678740	Pd(amphos)Cl ₂	887919-35-9	708.07	Yellow	Air Stable	X	X				
  697230	Pd(dppf)Cl ₂	72287-26-4	731.70	Red	Air Stable	X	X	X			
  379670	Pd(dppf)Cl ₂ · CH ₂ Cl ₂	95464-05-4	816.64	Red	Air Stable	X	X	X			
  701602	Pd(dtbpf)Cl ₂	95408-45-0	651.75	Brown	Air Stable		X		X		
  671916	Herrmann's Catalyst or cataCXium® C	172418-32-5	937.64	Light yellow	Air Stable				X		
  339768	Pd(MeCN) ₄ (BF ₄) ₂	21797-13-7	444.24	Dark Yellow	Air/Moisture Sensitive	X	X		X		X
  205877	PdBr ₂	13444-94-5	266.23	Dark Brown	Air Stable				X	X	X
  520659	PdCl ₂	7647-10-1	177.33	Red-Brown	Air Stable		X	X	X	X	

Palladium Catalysts and Precursors

	Structure and Cat. No.	Common Name	CAS No.	Mol. Wt.	Color	Stability	Negishi	Suzuki	Stille	Heck	Sonogashira	Buchwald-Hartwig
 NEW	 763403	RuPhos-Pd-G3	1445085-77-7	836.37	White	Air-Stable						X
 NEW	 761605	BrettPhos-Pd-G3	1470372-59-8	906.5	Beige	Air-Stable						X
 NEW	 762229	tBuXPhos-Pd-G3	1447963-75-8	794.37	Light Yellow	Air-Stable						X
 NEW	 763381	XPhos-Pd-G3	1445085-55-1	846.45	White	Air Stable		X				
 NEW	 762830	JackiePhos-Pd-G3	N/A	1166.4	White	Air Stable						X
 NEW	 669032	Pd-PEPPSI™-IPr	905459-27-0	679.46	Yellow	Air Stable	X	X			X	X
 NEW	 674702	Pd-PEPPSI™-SIPr	927706-57-8	681.47	Yellow	Air Stable	X	X				X
 NEW	 732117	Pd-PEPPSI™-IPent	1158652-41-5	791.67	Yellow	Air Stable	X	X	X			

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