

**Buchwald Portfolio –  
Precatalysts and Ligands**

Add  Aldrich

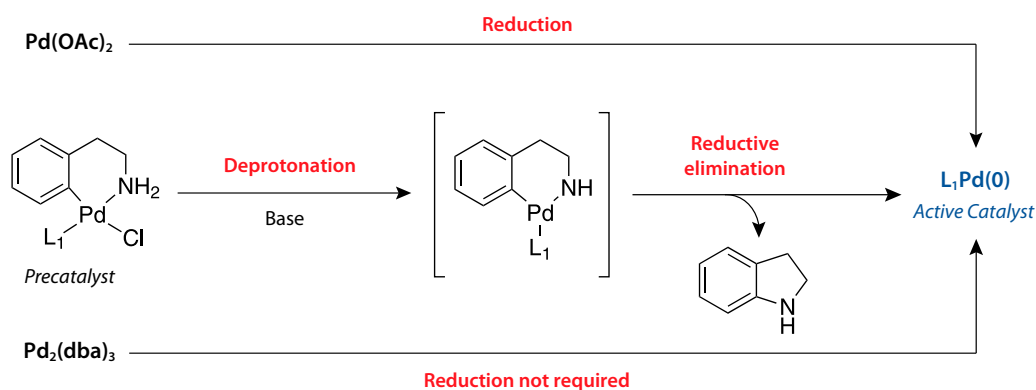
# Buchwald Precatalysts and Ligands

Dialkylbiaryl phosphine ligands, and the precatalysts derived from them, are commonly referred to as Buchwald Precatalysts and Ligands. These reagents have developed into a highly valuable class of compounds for palladium catalysis, and can now be used for a broad range of reactions. This brochure is designed to show the common uses and advantages of these powerful, and now commercially available, Buchwald Precatalysts and Ligands.

## Buchwald Precatalysts

### Different Pd Sources and Different Methods of Activation in C-N Cross Coupling Reactions

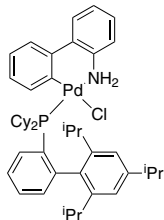
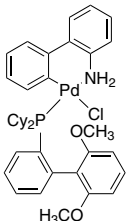
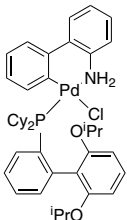
Buchwald Precatalysts are highly active for a range of Pd-catalyzed reactions. These bench-stable complexes can be activated under mildly basic conditions and provide a number of unique advantages over traditional palladium catalysts in terms of both activity and stability.



Precatalysts	$\text{Pd}(\text{OAc})_2$	$\text{Pd}_2(\text{dba})_3$
<b>Air stable</b>	<b>Air stable</b>	<b>Air stable</b>
<ul style="list-style-type: none"> <li>• Pd(II) complex</li> <li>• Efficient formation of active monoligated catalysts under basic reaction conditions, without reducing agent</li> <li>• Low catalyst loading</li> <li>• Short reaction time</li> </ul>	<ul style="list-style-type: none"> <li>• Pd(II) complex</li> <li>• Addition of exogenous reductant (<math>\text{NR}_3</math> or <math>\text{PhB}(\text{OH})_2</math>) or phosphine ligand for reduction of Pd(II)</li> <li>• High catalyst loading</li> <li>• Long reaction time</li> </ul>	<ul style="list-style-type: none"> <li>• Pd(0) complex</li> <li>• Without reducing agent</li> <li>• dba can bind Pd center and reduce catalytic activity</li> <li>• High catalyst loading</li> <li>• Long reaction time</li> </ul>

For bulk quantity inquiries contact: [catalysis@sial.com](mailto:catalysis@sial.com)

Structure	Cat. No.	Common Name	CAS No.	Mol. Wt.	Application for Pd Catalysis
	704954	XPhos Precatalyst	1028206-56-5	738.76	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of aldehydes</li> <li>• Buchwald-Hartwig amination</li> </ul>
	708739	tBuXPhos Precatalyst	1142811-12-8	686.69	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of acetate esters</li> <li>• Buchwald-Hartwig amination</li> </ul>
	704946	SPhos Precatalyst	1028206-58-7	760.72	<ul style="list-style-type: none"> <li>• Buchwald-Hartwig amination</li> </ul>
	707589	RuPhos Precatalyst	1028206-60-1	816.83	<ul style="list-style-type: none"> <li>• Buchwald-Hartwig amination</li> </ul>
	718750	BrettPhos Precatalyst	1148148-01-9	798.81	<ul style="list-style-type: none"> <li>• Buchwald-Hartwig amination</li> </ul>

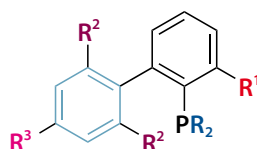
Structure	Cat. No.	Common Name	CAS No.	Mol. Wt.	Application for Pd Catalysis
	<b>741825</b> <i>New</i>	2 <sup>nd</sup> Generation XPhos Precatalyst	N/A	785.31	<ul style="list-style-type: none"> <li>• Suzuki coupling</li> <li>• Low temperature Buchwald-Hartwig amination</li> <li>• Heck coupling</li> </ul>
	<b>753009</b> <i>New</i>	2 <sup>nd</sup> Generation SPhos Precatalyst	N/A	719.19	<ul style="list-style-type: none"> <li>• Low temperature Buchwald-Hartwig amination</li> </ul>
	<b>753246</b> <i>New</i>	2 <sup>nd</sup> Generation RuPhos Precatalyst	N/A	775.25	<ul style="list-style-type: none"> <li>• Low temperature Buchwald-Hartwig amination</li> </ul>

# Buchwald Ligands

## Structural Features of Dialkylbiaryl Phosphine Ligands

**R<sup>2</sup>:** Increases catalyst stability by preventing cyclometalation, Encourages formation of L<sub>1</sub>Pd(0)

**R<sup>3</sup>:** When not equal to H, usually only for ease of synthesis



**R<sup>1</sup>:** Substitution promotes reductive elimination

**R:** Electron-rich groups accelerate rate of oxidative addition

: Prevents oxidation at P by O<sub>2</sub>, Accelerates reductive elimination

Structure	Cat. No.	Common Name	CAS No.	Mol. Wt.	Application for Pd Catalysis
	638099	Cyclohexyl JohnPhos	247940-06-3	350.48	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Negishi coupling</li> <li>Hiyama coupling</li> <li>Methylation of aryl halides</li> <li><math>\alpha</math>-Arylation of ketones</li> <li>Buchwald-Hartwig amination</li> <li>C-B bond formation</li> <li>Oxidation of alcohols to ketones and aldehydes</li> </ul>
	638021	DavePhos	213697-53-1	393.54	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Kumada-Corriu coupling</li> <li><math>\alpha</math>-Arylation of ketones</li> <li>Buchwald-Hartwig amination</li> <li>Rh-catalyzed hydroamination</li> </ul>
	638064	XPhos	564483-18-7	476.72	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Sonogashira coupling</li> <li>Hiyama coupling</li> <li>Stille coupling</li> <li>Carbonyl enolate coupling</li> <li>Buchwald-Hartwig amination</li> </ul>
	638072	SPhos	657408-07-6	410.53	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Kumada-Corriu coupling</li> <li>Negishi coupling</li> <li>Buchwald-Hartwig amination</li> </ul>
	695262	MePhos	251320-86-2	364.50	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li><math>\alpha</math>-Arylation of ketones</li> <li>Buchwald-Hartwig amination</li> </ul>
	663131	RuPhos	787618-22-8	466.64	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Negishi coupling</li> <li><math>\alpha</math>-Arylation reaction of oxindoles</li> <li>Buchwald-Hartwig amination</li> </ul>
	718742	BrettPhos	1070663-78-3	536.77	<ul style="list-style-type: none"> <li>Buchwald-Hartwig amination</li> <li>Trifluoromethylation of aryl chlorides</li> </ul>
	677280	<sup>s</sup> SPhos	1049726-96-6	512.57	<ul style="list-style-type: none"> <li>Suzuki coupling</li> <li>Rh-catalyzed 1,2-addition of arylboronic acids to aldehydes and ketones</li> </ul>

Structure	Cat. No.	Common Name	CAS No.	Mol. Wt.	Application for Pd Catalysis
	695882	PhDavePhos	240417-00-9	381.45	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of <math>\alpha</math>-amino acid esters</li> <li>• Heteroarene benzylation</li> <li>• Buchwald-Hartwig amination</li> </ul>
	638080	tBuXPhos	564483-19-8	424.64	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of tetramic acids</li> <li>• Decarboxylative coupling of aromatic acids and aryl iodides</li> <li>• Carboxylation of aryl bromides with CO<sub>2</sub></li> <li>• Buchwald-Hartwig amination</li> <li>• Buchwald-Hartwig C-O coupling</li> </ul>
	638439	JohnPhos	224311-51-7	298.40	<ul style="list-style-type: none"> <li>• Suzuki coupling</li> <li>• Heck coupling</li> <li>• Buchwald-Hartwig amination</li> <li>• Buchwald-Hartwig C-O coupling</li> <li>• C-Si bond formation</li> </ul>
	675938	Tetramethyl di-tBuXPhos	857356-94-6	480.75	<ul style="list-style-type: none"> <li>• Conversion of aryl halides to phenols</li> <li>• Buchwald-Hartwig amination</li> <li>• Buchwald-Hartwig C-O coupling</li> </ul>
	695211	tBuMePhos	255837-19-5	312.43	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of ketones</li> <li>• Buchwald-Hartwig C-O coupling</li> <li>• Formate reduction of <i>N</i>-heterocyclic allylic acetates</li> </ul>
	730998	tBuBrettPhos	1160861-53-9	484.69	<ul style="list-style-type: none"> <li>• Buchwald-Hartwig amination</li> <li>• C-F bond formation</li> <li>• <i>O</i>-Arylation of ethyl acetoxyhydroximate</li> <li>• Conversion of aryl and vinyl triflates to bromides and chlorides</li> <li>• Conversion of aryl chlorides, triflates, and nonaflates to nitroaromatics</li> </ul>
	695874	tBuDavePhos	224311-49-3	341.47	<ul style="list-style-type: none"> <li>• <math>\alpha</math>-Arylation of esters</li> <li>• Buchwald-Hartwig C-O coupling</li> <li>• Coupling of ammonia with aryl halides</li> <li>• C-Si bond formation</li> </ul>
	731013	JackiePhos	1160861-60-8	796.66	<ul style="list-style-type: none"> <li>• <i>N</i>-arylation of secondary amides</li> </ul>

## References:

- Surry, D. S.; Buchwald, S. L. *Chem. Sci.* **2011**, *2*, 27-50.  
 Martin, R.; Buchwald, S. L. *Acc. Chem. Res.* **2008**, *41*, 1461-1473.  
 Surry, D. S.; Buchwald, S. L. *Angew. Chem. Int. Ed.* **2008**, *47*, 6338-6361.

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