

**Buchwald Portfolio:  
Palladacycles and Ligands**

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ALDRICH

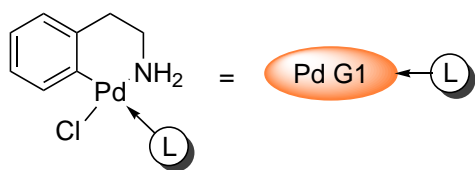
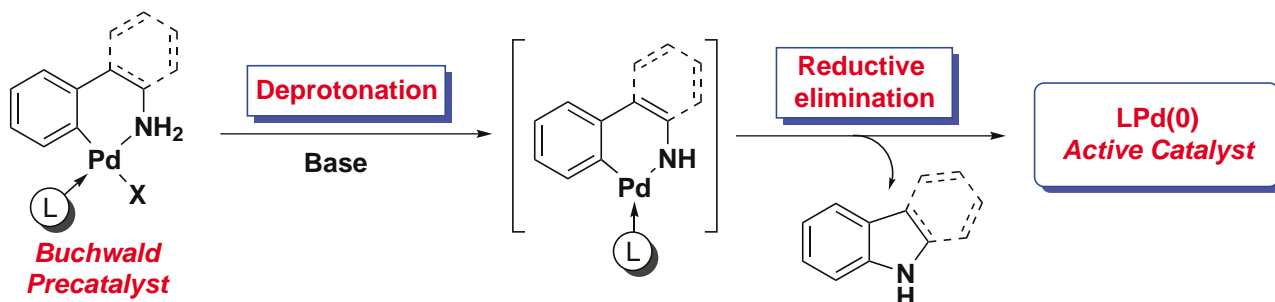
## Introduction

The Buchwald group has developed a series of highly active and versatile palladium precatalysts and biarylphosphine ligands used in cross-coupling reactions for the formation of C-C, C-N, C-O, C-F, C-CF<sub>3</sub>, and C-S bonds. The ligands are electron-rich, and highly tunable to provide catalyst systems with a diverse scope, high stability, and reactivity.

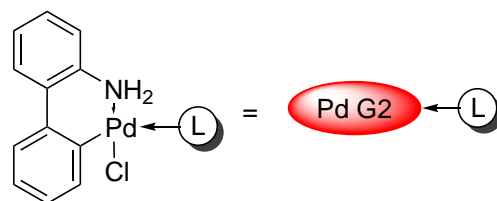
The corresponding Buchwald precatalysts are air, moisture, and thermally-stable and display good solubility in common organic

solvents. The use of these precatalysts in cross-coupling reactions typically allows the researcher to use lower catalyst loadings, and results in shorter reaction times. Additionally, their use ensures the efficient formation of the active catalytic species, generally without reducing agents, and allows one to accurately control the ligand:palladium ratio. The unique features of the precatalysts have led to the discovery of new methods that would not otherwise be feasible using traditional Pd sources.

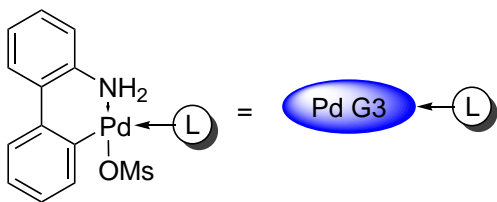
The ligands, precatalysts and methodology developed in the Buchwald group are user friendly and have rendered previously difficult cross couplings reactions much easier to achieve.



The formation of the active Pd(0) species in the first generation (G1) precatalysts is easy to generate, requiring merely a deprotonation with base. The resulting catalyst is very active, even at temperatures down to -40 °C, and can be used in a variety of cross coupling protocols.

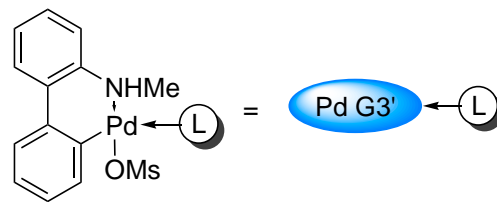


The second generation (G2) precatalysts substituted the phenethylamine based backbone of the (G1) complex with a biphenyl-based ligand. This improvement on the previous generation allows the researcher to create the active Pd species at room temperature with weak phosphate or carbonate bases. These catalysts prove remarkably adept at achieving a variety of Suzuki-Miyaura couplings among other cross-coupling reactions.



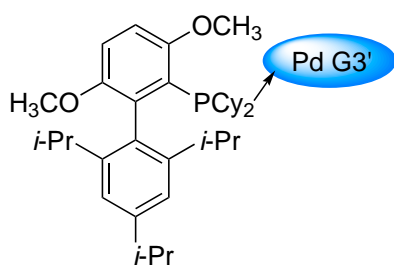
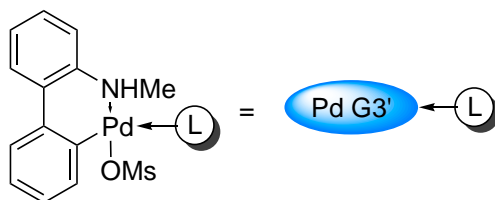
The third generation (G3) precatalysts are the most versatile yet, as they are highly soluble in a wide variety of common organic solvents and are able to accommodate very bulky ligands such as the BrettPhos family. Furthermore these catalysts show remarkably long life in solution.

References listed on page 14.

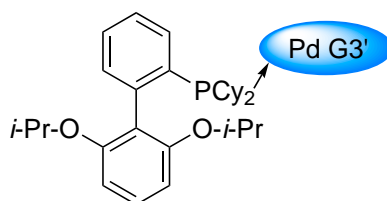


In some rare cases, the carbazole leaving group can inhibit the catalyst in a reaction. To circumvent this issue, the Buchwald group has prepared a modified G3 precatalyst (G3') by methylating the amino group on the biphenyl backbone. These G3' precatalysts exhibit higher solubilities in cross-coupling reactions while maintaining excellent catalytic activity.

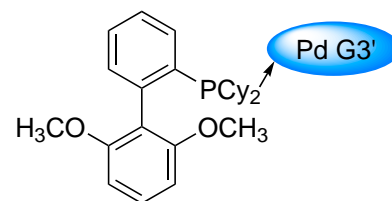
# G3' Complexes



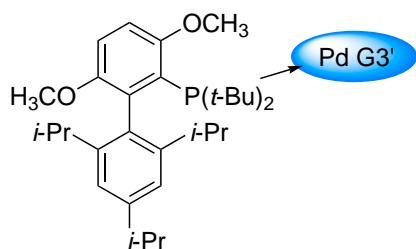
**804355\***  
*N*-MeBrettPhos Pd G3  
 MW: 920.54  
 250 mg; 1 g



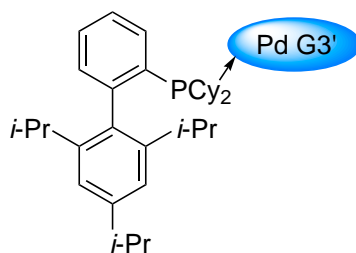
**804290\***  
*N*-MeRuPhos Pd G3  
 MW: 850.40  
 250 mg; 1 g



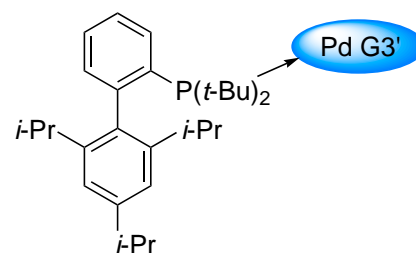
**804282\***  
*N*-MeSPhos Pd G3  
 MW: 794.30  
 100 mg; 1 g



**807877\***  
*N*-MeTBuBrettPhos Pd G3  
 MW: 868.46  
 100 mg; 500 mg



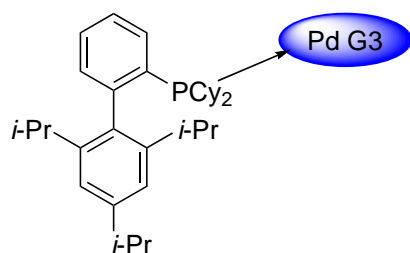
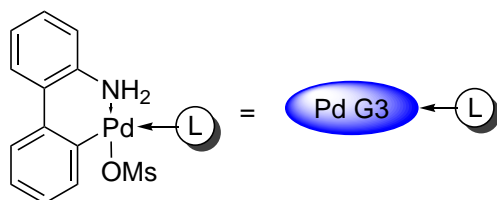
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*N*-MeXPhos Pd G3  
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 250 mg; 1 g



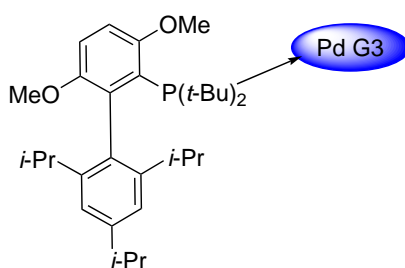
**804262\***  
*N*-MeTBuXPhos Pd G3  
 MW: 808.41  
 250 mg; 1 g

\*Coming Soon

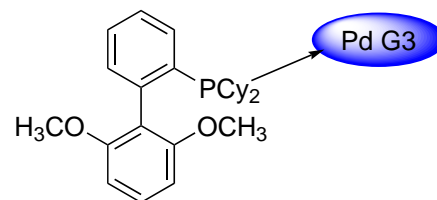
## G3 Complexes



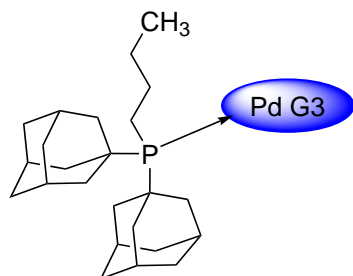
**763381**  
 XPhos Pd G3  
 1445085-55-1  
 MW: 846.45  
 250 mg; 1 g; 5 g



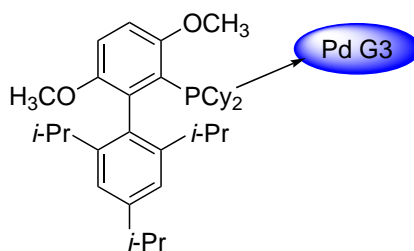
**745979**  
 tBuBrettPhos Pd G3  
 MW: 854.43  
 100 mg; 500 mg; 1 g; 5 g



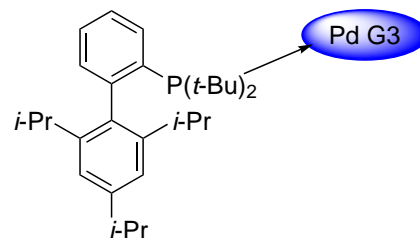
**776246**  
 SPhos Pd G3  
 MW: 780.26  
 250 mg; 1 g; 5 g



**761435**  
 cataCXium A Pd G3  
 MW: 728.27  
 250 mg; 1 g; 5 g

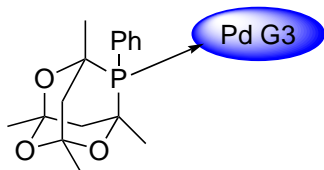


**761605**  
 BrettPhos Pd G3  
 1470372-59-8  
 MW: 906.50  
 250 mg; 1 g; 5 g; 10 g



**762229**  
 tBuXPhos Pd G3  
 1447963-75-8  
 MW: 794.37  
 250 mg; 1 g; 5 g

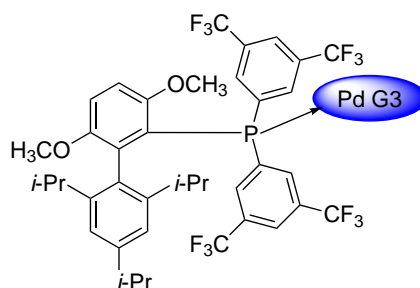
# G3 Complexes


**762822**

[(1,3,5,7-Tetramethyl-6-phenyl-2,4,6-trioxa-6-phosphaadamantane)-2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate

MW: 662.04

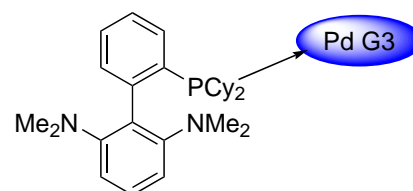
500 mg; 2 g


**762830**

JackiePhos Pd G3

MW: 1166.40

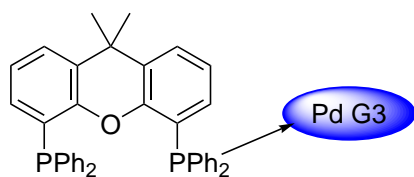
100 mg; 500 mg; 1 g; 5 g


**763004**

CPhos Pd G3

MW: 806.34

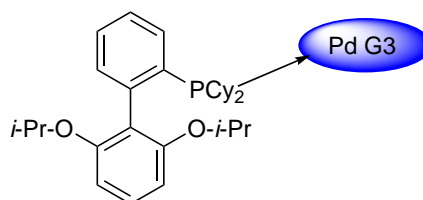
100 mg; 500 mg; 1 g; 5 g


**763039**

XantPhos Pd G3

MW: 948.35

250 mg; 1 g; 5 g

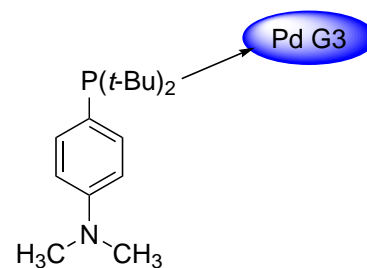

**763403**

RuPhos Pd G3

1445085-77-7

MW: 836.37

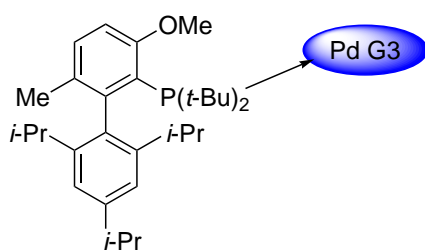
250 mg; 1 g; 5 g


**764183**

APHOS Pd G3

MW: 635.11

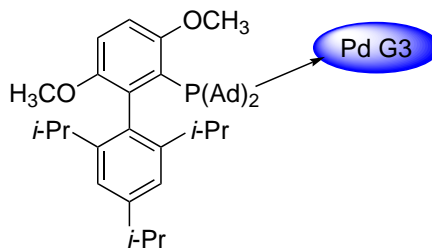
250 mg; 1 g; 5 g


**773905**

RockPhos Pd G3

MW: 838.43

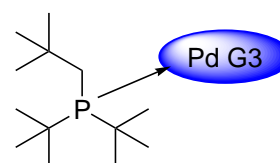
100 mg; 500 mg; 1 g; 5 g


**776106**

AdBrettPhos Pd G3

MW: 1010.65

100 mg; 500 mg; 2 g; 5 g

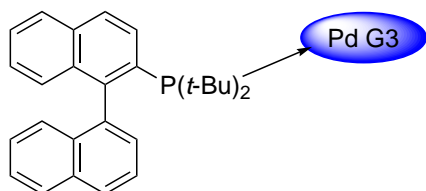

**794201**

 Neopentyl(*t*Bu)<sub>2</sub>P Pd G3

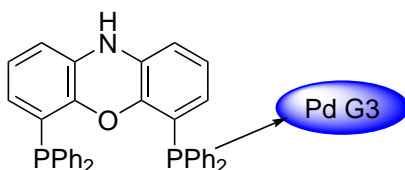
MW: 586.08

250 mg; 1 g

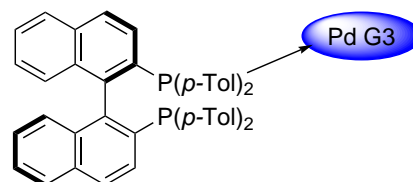
## G3 Complexes



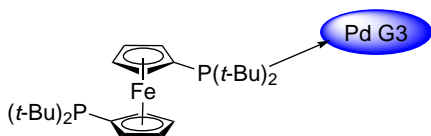
796530  
TrixiePhos Pd G3  
MW: 768.25  
250 mg; 1 g



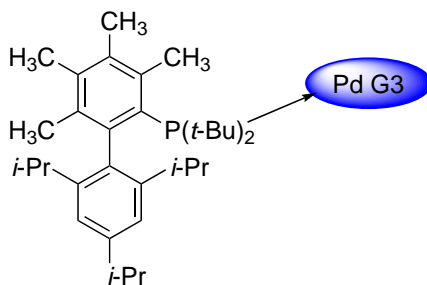
794228  
N-XantPhos Pd G3  
MW: 921.29  
250 mg; 1 g



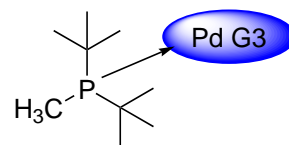
RNI00178  
(R)-TolBINAP Pd G3  
MW: 1048.51  
250 mg



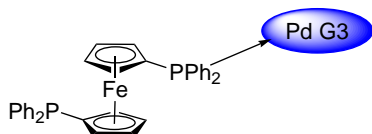
804975\*  
DTBPF Pd G3  
MW: 844.15  
250 mg



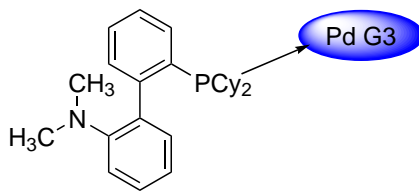
RNI00184  
Me<sub>4</sub>tBuXPhos Pd G3  
MW: 850.48  
250 mg



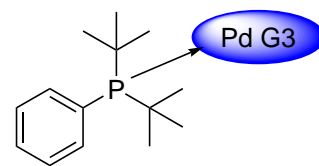
RNI00185  
(tBu)<sub>2</sub>PMe Pd G3  
MW: 529.97  
250 mg



804983\*  
DPPF Pd G3  
MW: 954.18  
250 mg



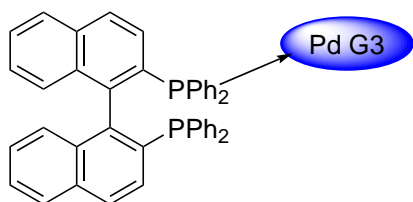
804959\*  
DavePhos Pd G3  
MW: 763.28  
250 mg



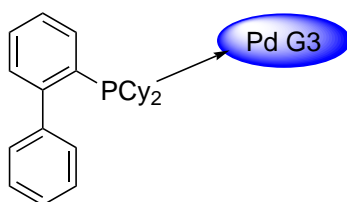
RNI00188  
(tBu)<sub>2</sub>PPh Pd G3  
MW: 592.04  
250 mg

\*Coming Soon

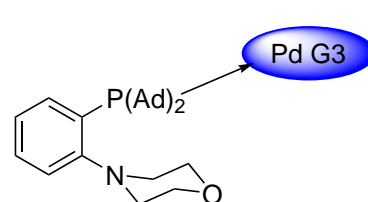
## G3 Complexes



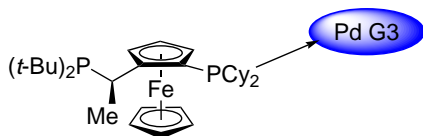
804967\*  
*rac*-BINAP Pd G3  
MW: 992.40  
100 mg



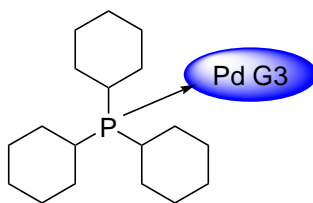
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CyJohnPhos Pd G3  
MW: 720.21  
250 mg



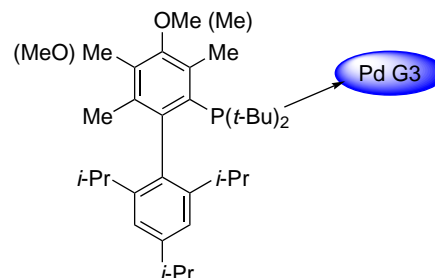
792357  
MorDalPhos Pd G3  
MW: 833.37  
500 mg; 2 g; 5 g



747130  
Josiphos SL-J009-1 Pd G3  
MW: 924.28  
100 mg; 250 mg; 1 g; 5 g



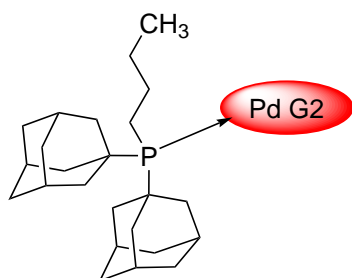
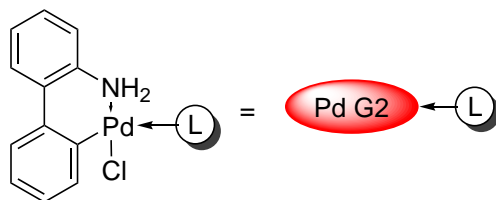
764175  
PCy<sub>3</sub> Pd G3  
MW: 650.16  
250 mg; 1 g; 5 g



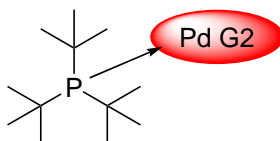
804193\*  
Me<sub>3</sub>(OMe)tBuXPhos Pd G3  
MW: 866.49  
1 g; 5 g

\*Coming Soon

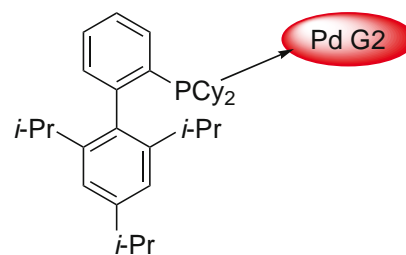
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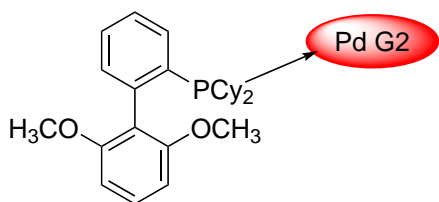
**761311**  
cataCXium A Pd G2  
1375477-29-4  
MW: 668.63  
250 mg; 1 g; 5 g



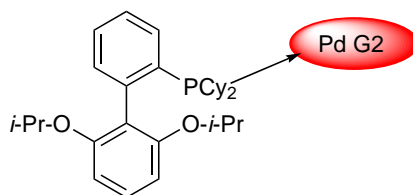
**756482**  
P(*t*-Bu)<sub>3</sub> Pd G2  
1375325-71-5  
MW: 512.40  
500 mg; 2 g; 5 g



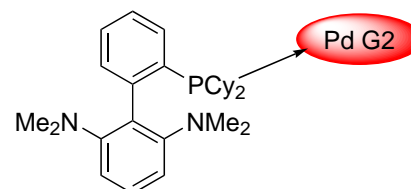
**741825**  
XPhos Pd G2  
1310584-14-5  
MW: 786.80  
250 mg; 1 g; 5 g; 10 g; 25 g; 100 g; 500 g



**753009**  
SPhos Pd G2  
1375325-64-6  
MW: 720.62  
250 mg; 1 g; 5 g



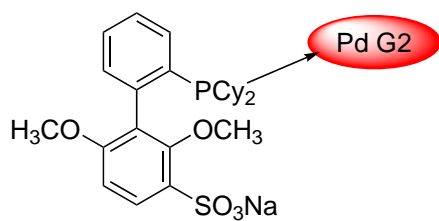
**753246**  
RuPhos Pd G2  
1375325-68-0  
MW: 776.72  
250 mg; 1 g; 5 g



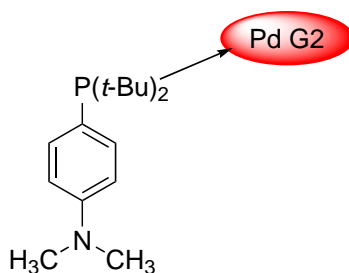
**763012**  
CPhos Pd G2  
MW: 746.70  
100 mg; 500 mg



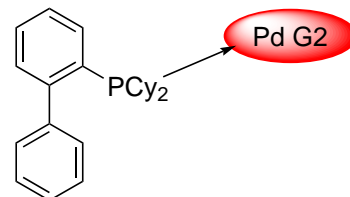
## G2 Complexes



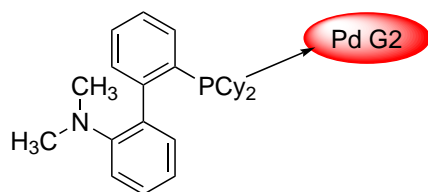
**763314**  
sSPhos Pd G2  
(water soluble SPhos)  
MW: 822.66  
100 mg; 500 mg



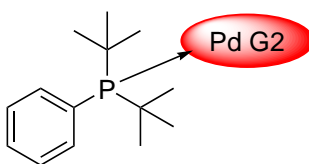
**764299**  
APHos Pd G2  
MW: 575.46  
500 mg; 2 g



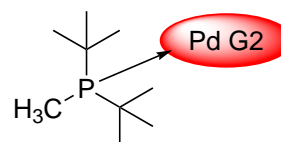
**747807**  
CyJohnPhos Pd G2  
MW: 660.56  
500 mg; 1 g



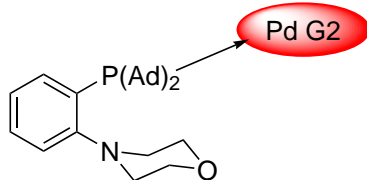
**RNI00181**  
DavePhos Pd G2  
MW: 703.63  
250 mg



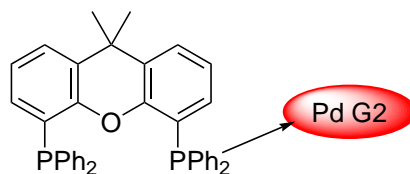
**RNI00182**  
(tBu)<sub>2</sub>PPh Pd G2  
MW: 532.39  
250 mg



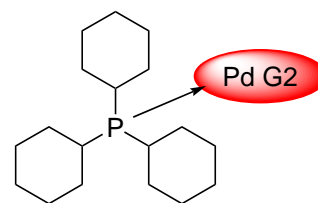
**RNI00183**  
(tBu)<sub>2</sub>PMe Pd G2  
MW: 470.32  
250 mg



**792349**  
MorDalphos Pd G2  
MW: 773.72  
500 mg; 2 g

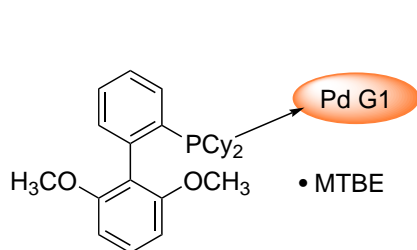
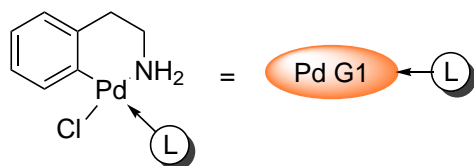


**763047**  
XantPhos Pd G2  
1375325-77-1  
MW: 888.71  
500 mg; 2 g; 5 g

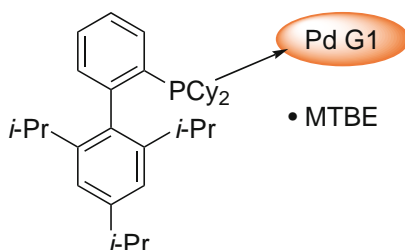


**756741**  
PCy<sub>3</sub> Pd G2  
MW: 590.52  
1 g; 5 g

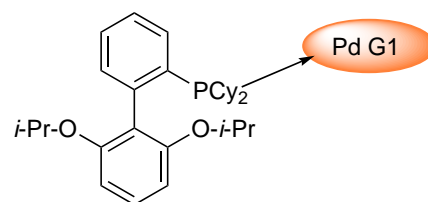
## G1 Complexes



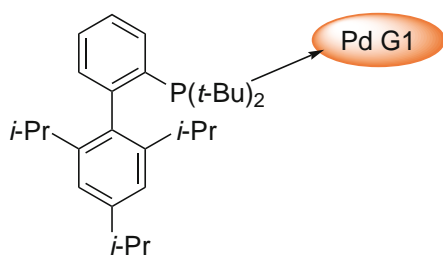
704946  
SPhos Pd G1  
1028206-58-7  
MW: 760.72  
250 mg; 1 g



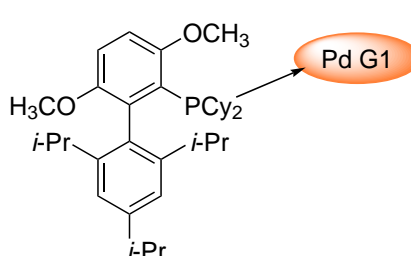
704954  
XPhos Pd G1  
1028206-56-5  
MW: 738.76  
250 mg; 1 g



707589  
RuPhos Pd G1  
1028206-60-1  
MW: 816.83  
250 mg; 1 g



708739  
tBuXPhos Pd G1  
1142811-12-8  
MW: 686.69  
250 mg; 1 g

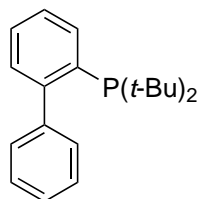


718750  
BrettPhos Pd G1  
1148148-01-9  
MW: 798.81  
100 mg; 1 g

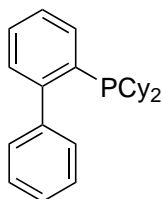


741868  
Buchwald Palladacycle Precatalyst Kit  
(G1 complexes)  
250 mg XPhos, 704954  
250 mg SPhos, 704946  
100 mg RuPhos, 707589  
100 mg tBuXPhos, 708739  
100 mg BrettPhos, 718750

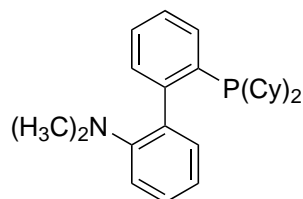
# Buchwald Ligands



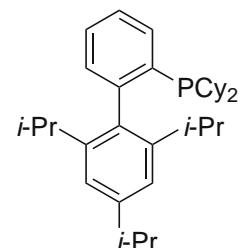
**638439**  
 JohnPhos  
 224311-51-7  
 MW: 298.40  
 1 g; 5 g; 25 g; 100 g



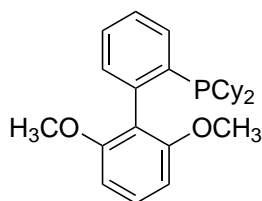
**638099**  
 CyJohnPhos  
 247940-06-3  
 MW: 350.48  
 1 g; 5 g; 25 g



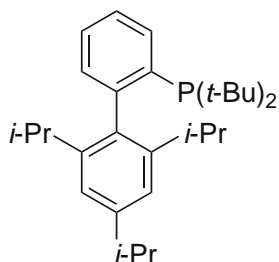
**638021**  
 DavePhos  
 213697-53-1  
 MW: 393.54  
 1 g; 5 g; 25 g; 100 g



**638064**  
 XPhos  
 564483-18-7  
 MW: 476.72  
 1 g; 5 g; 25 g; 100 g; 500 g



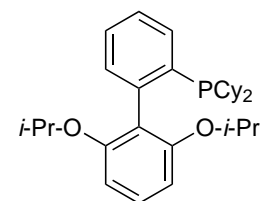
**638072**  
 SPhos  
 657408-07-6  
 MW: 410.53  
 1 g; 5 g; 25 g; 500 g



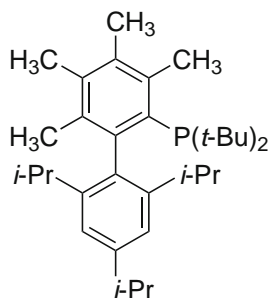
**638080**  
 tBuXPhos  
 564483-19-8  
 MW: 424.64  
 1 g; 5 g; 25 g; 100 g; 500 g



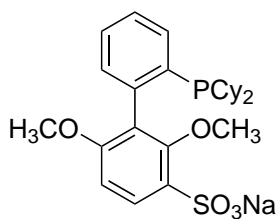
**659932**  
 Buchwald Ligands Kit I  
 1 g JohnPhos, **638439**  
 1 g CyJohnPhos, **638099**  
 1 g XPhos, **638064**  
 1 g tBuXPhos, **638080**  
 1 g SPhos, **638072**  
 1 g DavePhos, **638021**



**663131**  
 RuPhos  
 787618-22-8  
 MW: 466.64  
 1 g; 5 g; 25 g; 100 g



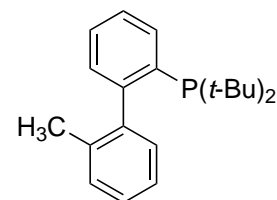
**675938**  
 Me<sub>4</sub>tBuXPhos  
 857356-94-6  
 MW: 480.75  
 250 mg; 1 g; 5 g



**677280**  
 sSPhos  
 1049726-96-6  
 MW: 512.57 (anh. basis)  
 500 mg; 2 g



**687243**  
 Buchwald Ligands Kit II  
 1 g JohnPhos, **638439**  
 1 g CyJohnPhos, **638099**  
 1 g XPhos, **638064**  
 1 g tBuXPhos, **638080**  
 1 g SPhos, **638072**  
 1 g DavePhos, **638021**  
 1 g RuPhos, **663131**  
 500 mg sSPhos, **677280**  
 250 mg Me<sub>4</sub>tBuXPhos, **675938**



**695211**  
 tBuMePhos  
 255837-19-5  
 MW: 312.43  
 1 g

# Buchwald Ligands



**698903**

Buchwald Ligands Kit III

1 g JohnPhos, **638439**

1 g CyJohnPhos, **638099**

1 g XPhos, **638064**

1 g *t*BuXPhos, **638080**

1 g SPhos, **638072**

1 g DavePhos, **638021**

1 g RuPhos, **663131**

500 mg *s*SPhos, **677280**

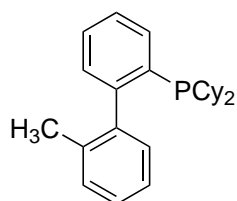
250 mg Me<sub>2</sub>*t*BuXPhos, **675938**

1 g *t*BuMePhos, **695211**

1 g MePhos, **695262**

1 g *t*BuDavePhos, **695874**

1 g PhDavePhos, **695882**



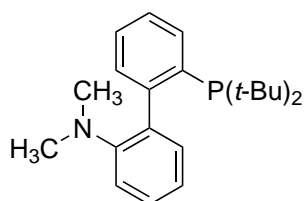
**695262**

MePhos

251320-86-2

MW: 364.50

1 g; 5 g



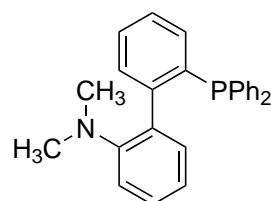
**695874**

*t*BuDavePhos

224311-49-3

MW: 341.47

1 g; 5 g



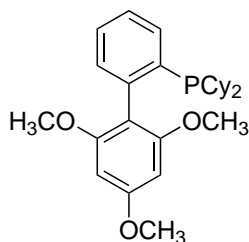
**695882**

PhDavePhos

240417-00-9

MW: 381.45

1 g; 5 g



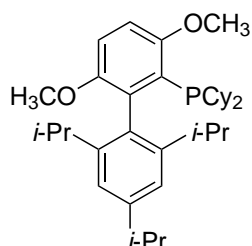
**707430**

2'-Dicyclohexylphosphino-  
2,4,6-trimethoxybiphenyl

1000171-05-0

MW: 440.55

1 g; 5 g



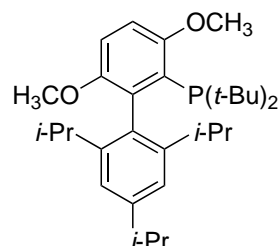
**718742**

BrettPhos

1070663-78-3

MW: 536.77

100 mg; 500 mg; 1 g; 5 g; 50 g



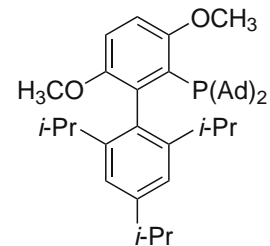
**730998**

*t*BuBrettPhos

1160861-53-9

MW: 484.69

100 mg; 500 mg; 5 g; 50 g



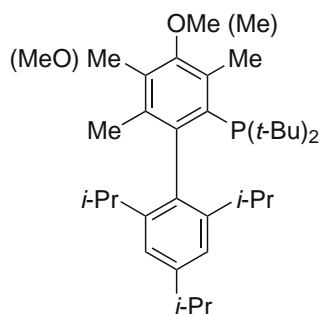
**768154**

AdBrettPhos

1160861-59-5

MW: 640.92

100 mg; 500 mg; 1 g

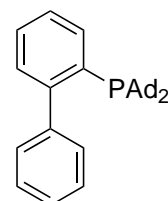


**792470**

Me<sub>3</sub>(OMe)*t*BuXPhos

MW: 496.75

250 mg 1 g; 5 g



**767689**

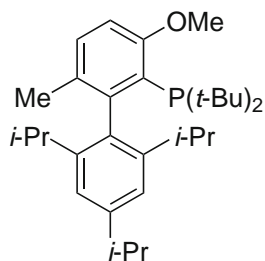
(2-Biphenyl)di-1-adamantylphosphine

224311-55-1

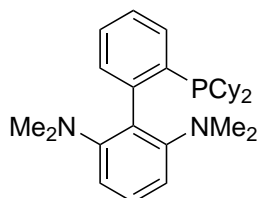
MW: 454.63

250 mg; 1 g

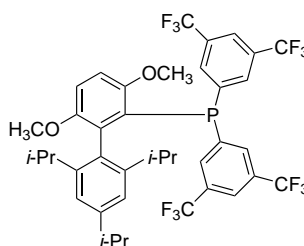
## Related Ligands



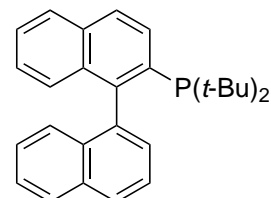
**791016**  
 RockPhos  
 1262046-34-3  
 MW: 468.69  
 500 mg; 2 g



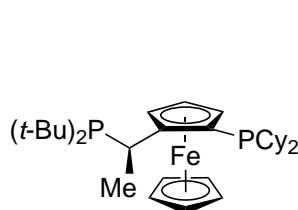
**759171**  
 CPhos  
 1160556-64-8  
 MW: 436.61  
 1 g; 5 g



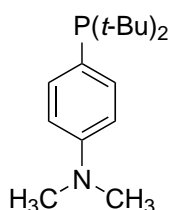
**731013**  
 JackiePhos  
 1160861-60-8  
 MW: 796.66  
 100 mg; 250 mg; 1 g



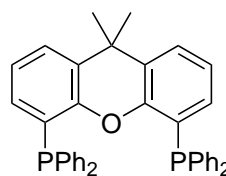
**710342**  
 TrixiePhos  
 255836-67-0  
 MW: 398.52  
 500 mg



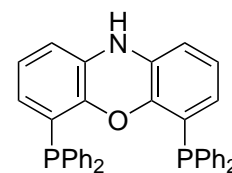
**88733**  
 Josiphos SL-J009-1  
 158923-11-6  
 MW: 554.55  
 100 mg; 500 mg; 1 g; 5 g



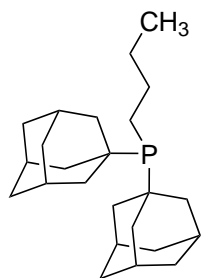
**677264**  
 APhos  
 932710-63-9  
 MW: 265.37  
 1 g; 5 g



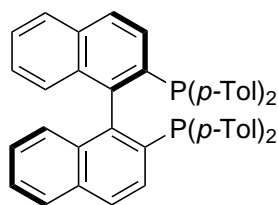
**526460**  
 XantPhos  
 161265-03-8  
 MW: 578.62  
 1 g; 5 g; 25 g



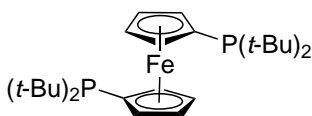
**666564**  
 N-XantPhos  
 (4,6-Bis(diphenylphosphino)  
 phenoxazine)  
 261733-18-0  
 MW: 551.55  
 500 mg; 1 g



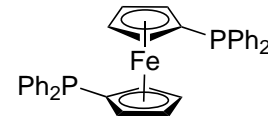
**671479**  
 cataCXium A  
 321921-71-5  
 MW: 358.54  
 1 g; 5 g; 50 g; 100 g; 250 g



**693049**  
 (R)-Tol-BINAP  
 99646-28-3  
 MW: 678.78  
 100 mg; 500 mg

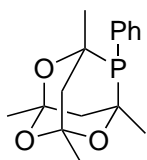


**695149**  
 DTBPF  
 1,1'-Bis(di-tert-  
 butylphosphino)ferrocene  
 84680-95-5  
 MW: 474.42  
 250 mg; 1 g

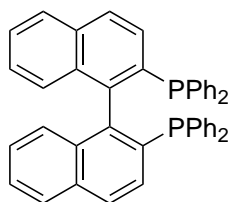


**177261**  
 DPPF  
 1,1'-Bis(diphenylphosphino)  
 ferrocene  
 12150-46-8  
 MW: 554.38  
 1 g; 10 g; 25 g; 250 g

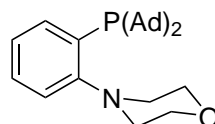
## Related Ligands



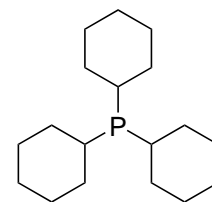
**695459**  
1,3,5,7-Tetramethyl-6-phenyl-2,4,8-trioxo-6-phosphaadamantane  
97739-46-3  
MW: 292.31  
500 mg; 2 g



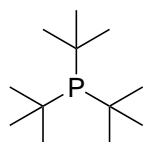
**481084**  
*rac*-BINAP  
2,2'-Bis(diphenylphosphino)-1,1'-binaphthalene  
98327-87-8  
MW: 622.67  
5 g; 25 g; 100 g; 500 g



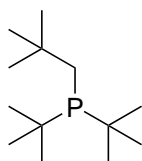
**751618**  
MorDalPhos  
Di(1-adamantyl)-2-morpholinophenylphosphine  
1237588-12-3  
MW: 463.63  
250 mg; 1 g



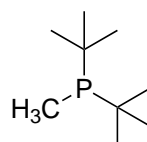
**261971**  
Tricyclohexylphosphine  
2622-14-2  
MW: 280.43  
1 g; 5 g; 25 g; 250 g



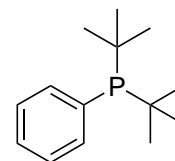
**570958**  
Tri-*tert*-butylphosphine  
13716-12-6  
MW: 202.32  
1 g; 5 g; 10 g



**676187**  
Di-*tert*-butylneopentylphosphine  
60633-21-8  
MW: 216.34  
1 g



**642629**  
Di-*tert*-butylmethylphosphine  
6002-40-0  
MW: 160.24  
5 g



**682411**  
Di-*tert*-butylphenylphosphine  
32673-25-9  
MW: 222.31  
1 g; 5 g

### Selected References:

#### Precatalyst Review

Bruneau, A. et al. *ACS Catal.* **2015**, *5*, 1386.

#### First Generation Precatalysts

Biscoe, M. R.; Fors, B. P.; Buchwald, S. L. *J. Am. Chem. Soc.* **2008**, *130*, 6686.

#### Second Generation Precatalysts

Kinzel, T.; Zhang, Y.; Buchwald, S. L. *J. Am. Chem. Soc.* **2010**, *132*, 14073.

#### Third Generation Precatalysts

Bruno, N. C.; Niljianskul, N.; Buchwald, S. L. *J. Org. Chem.* **2014**, *79*, 4161.

Yang, Y. et al. *Org. Lett.* **2014**, *16*, 4638.

Duefert, A.; Billingsley, K.; Buchwald, S. L. *J. Am. Chem. Soc.* **2013**, *135*, 12877.

Name	Ligand	G1 Complex	G2 Complex	G3 Complex	G3' complex
<b>BrettPhos</b>	718742	718750	—	761605	804355*
AdBrettPhos	768154	—	—	776106	—
tBuBrettPhos	730998	—	—	745979	807877*
<b>DavePhos</b>	638021	—	RNI00181	804959*	—
tBuDavePhos	695874	—	—	—	—
PhDavePhos	695882	—	—	—	—
<b>JohnPhos</b>	638439	—	—	—	—
CyJohnPhos	638099	—	747807	RNI00192	—
<b>MePhos</b>	695262	—	—	—	—
tBuMePhos	695211	—	—	—	—
RuPhos	663131	707589	753246	763403	804290*
<b>SPhos</b>	638072	704946	753009	776246	804282*
sSPhos	677280	—	763314	—	—
<b>XPhos</b>	638064	704954	741825	763381	804274*
tBuXPhos	638080	708739	—	762229	804266*
Me <sub>3</sub> (OMe)tBuXPhos	792470	—	—	804193*	—
Me <sub>4</sub> tBuXPhos	675938	—	—	RNI00184	—
(2-Biphenyl)di-1-adamantylphosphine	767689	—	—	—	—
2'-Dicyclohexylphosphino-2,4,6-trimethoxybiphenyl	707430	—	—	—	—
<b>Select Non-Buchwald Ligands</b>					
APhos	677264	—	764299	764183	—
rac-BINAP	481084	—	—	804967*	—
P( <i>t</i> -Bu) <sub>3</sub>	570958	—	756482	—	—
( <i>t</i> Bu) <sub>2</sub> PMe	642629	—	RNI00183	RNI00185	—
( <i>t</i> Bu) <sub>2</sub> PPh	682411	—	RNI00182	RNI00188	—
cataCXium A	671479	—	761311	761435	—
CPhos	759171	—	763012	763004	—
PCy <sub>3</sub>	261971	—	756741	764175	—
DPPF	177261	—	—	804983*	—
DTBPF	695149	—	—	804975*	—
JackiePhos	731013	—	—	762830	—
Josphos SL-J009-1	88733	—	—	747130	—
MorDalPhos	751618	—	792349	792357	—
Neopentyl( <i>t</i> Bu) <sub>2</sub> P Pd G3	676187	—	—	794201	—
RockPhos	791016	—	—	773905	—
1,3,5,7-Tetramethyl-6-phenyl-2,4,6-trioxa-6-phosphaadamantane	695459	—	—	762822	—
( <i>R</i> )-Tol-BINAP	693049	—	—	RNI00178	—
TrixiePhos	710342	—	—	796530	—
XantPhos	526460	—	763047	763039	—
<i>N</i> -XantPhos	666564	—	—	794228	—

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