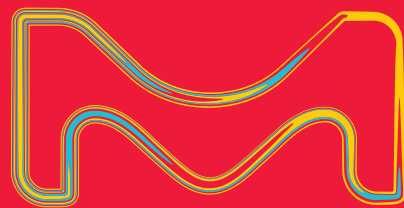


Sigma-Aldrich®

Lab Materials & Supplies

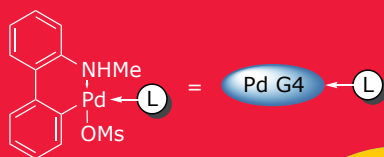
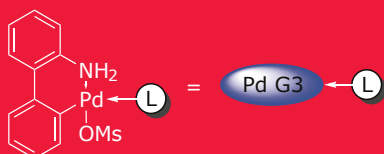
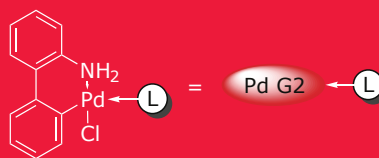
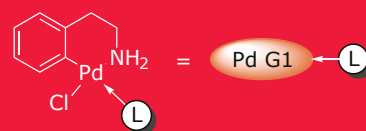


Buchwald系列产品

环钯化合物与配体

《交叉偶联反应指南》

下载链接: aldrich.com/cc-guide

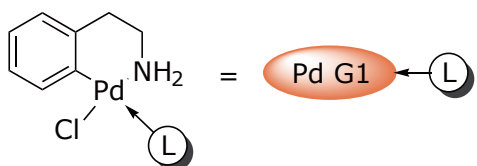
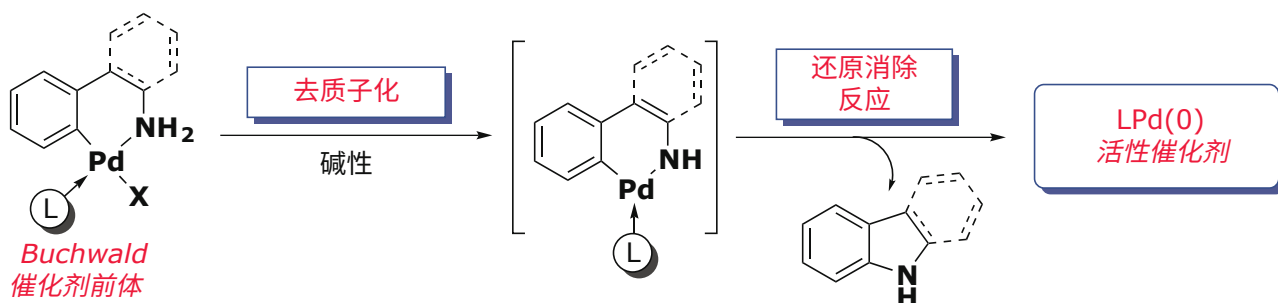


引言

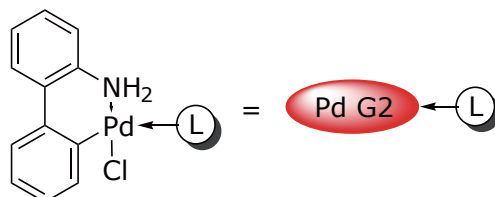
Buchwald团队已开发出一系列高活性的通用型钯催化剂前体和膦配体,用于交叉偶联反应以形成C-C、C-N、C-O、C-F、C-CF₃和C-S键。这些配体的富电子和高度可调性,使催化剂系统具有广泛的适用性、高稳定性和高活性。

Buchwald催化剂前体具有空气、潮湿和热稳定性,可良好地溶解于常用有机溶剂。在交叉偶联反应中使用这些催化剂前体,通常可减少催化剂用量并缩短反应时间;同时,也能确保活性催化物的形成,一般不需要使用还原剂,并且能够准确控制配体与钯的比例。该催化剂前体的独特之处使人们发现了新方法,这是使用传统Pd源所不能实现的。

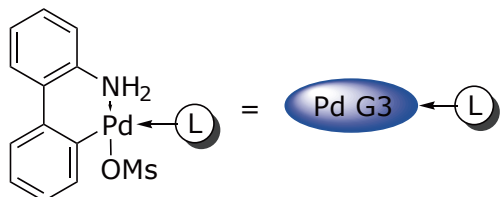
Buchwald团队开发的配体、催化剂前体和方法学非常人性化,使之前难以完成的交叉偶联反应更容易实现。



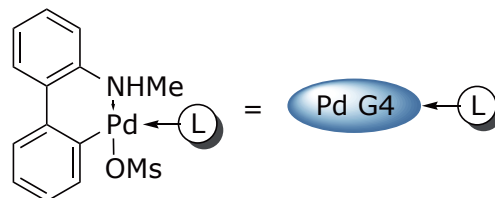
第一代 (G1) 催化剂前体中的活性Pd (0) 类易于生成,只需在碱性条件下去质子化。所得催化剂活性非常高,即使是在-40°C的低温下,适用于多种交叉偶联反应。



第二代 (G2) 催化剂前体以联苯配体取代了 (G1) 复合物的苯乙胺骨架。经过这一改进,研究人员在室温下使用弱磷酸盐或碳酸盐即可生成活性Pd类。这类催化剂明显更适用于完成其他交叉偶联反应中大量的Suzuki-Miyaura偶联。

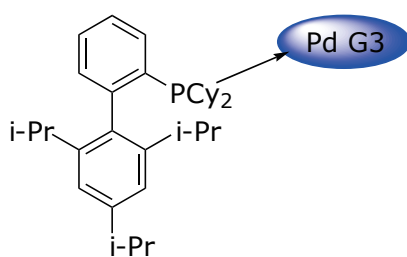
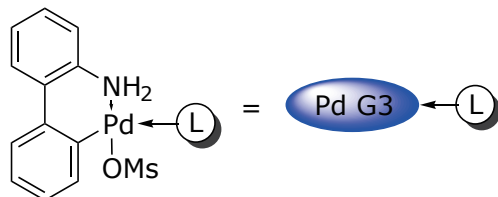


第三代 (G3) 催化剂前体的通用性最强,可高度溶解于多种常用有机溶剂,并且能够容纳大量配体,如BrettPhos家族。此外,这类催化剂在溶液中的效力显著延长。

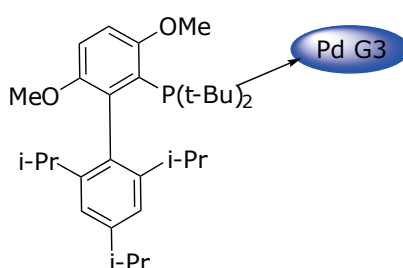


在一些稀有情况下,唑啉离去基团可抑制反应中的催化剂。为避免这类问题发生,Buchwald团队通过对联苯骨架上的氨基进行甲基化,制备出改进型G3催化剂前体 (G4)。G4催化剂前体在交叉偶联反应中具有更高的溶解性,同时也保留了G3催化剂卓越的催化活性。

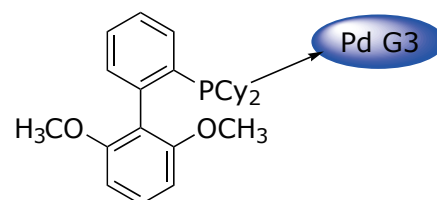
G3 Complexes



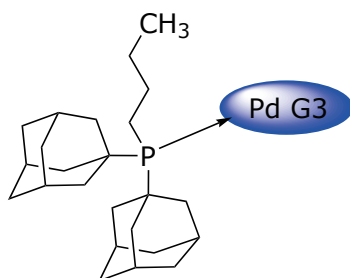
763381
XPhos Pd G3
1445085-55-1
MW: 846.45
250 mg; 1 g; 5 g



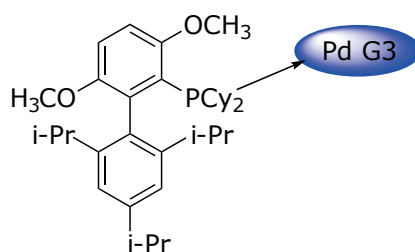
745979
tBuBrettPhos Pd G3
MW: 854.43
100 mg; 500 mg; 1 g; 5 g



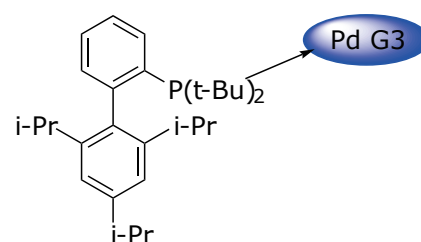
776246
SPhos Pd G3
MW: 780.26
250 mg; 1 g; 5 g



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

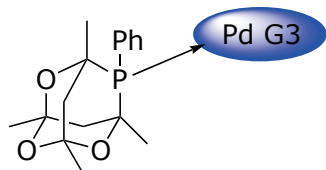


761605
BrettPhos Pd G3
1470372-59-8
MW: 906.50
250 mg; 1 g; 5 g; 10 g



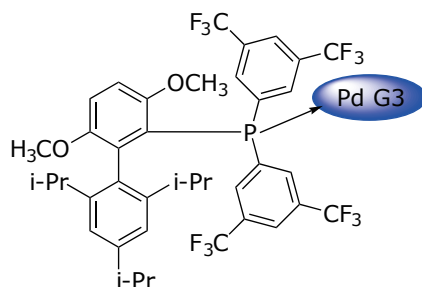
762229
tBuXPhos Pd G3
1447963-75-8
MW: 794.37
250 mg; 1 g; 5 g

G3 Complexes



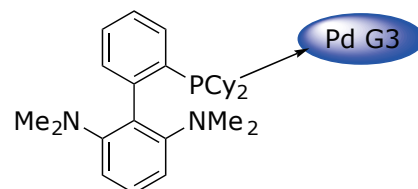
762822

[(1,3,5,7-Tetramethyl-6-phenyl-2,4,6-trioxo-6-phosphaadamantane)-2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate
MW: 662.04
500 mg; 2 g



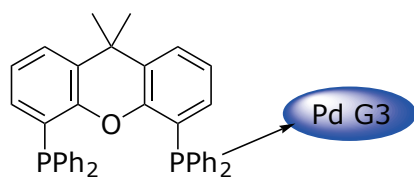
762830

JackiePhos Pd G3
MW: 1166.40
100 mg; 500 mg; 1 g; 5 g



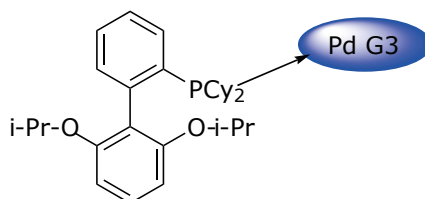
763004

CPhos Pd G3
MW: 806.34
100 mg; 500 mg; 1 g; 5 g



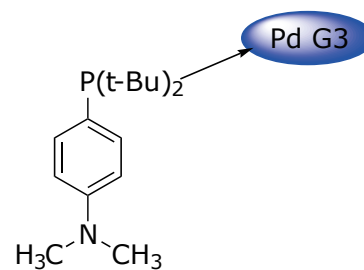
763039

XantPhos Pd G3
MW: 948.35
250 mg; 1 g; 5 g



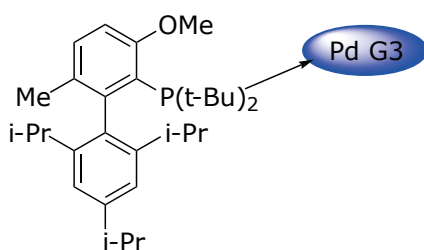
763403

RuPhos Pd G3
1445085-77-7
MW: 836.37
250 mg; 1 g; 5 g



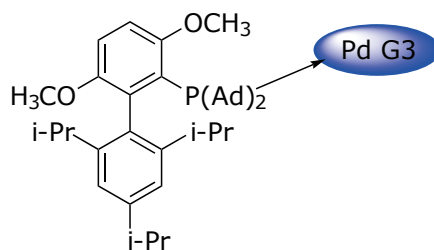
764183

APhos Pd G3
MW: 635.11
250 mg; 1 g; 5 g



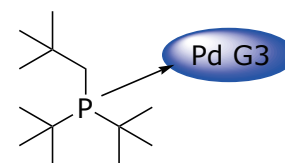
773905

RockPhos Pd G3
MW: 838.43
100 mg; 500 mg; 1 g; 5 g



776106

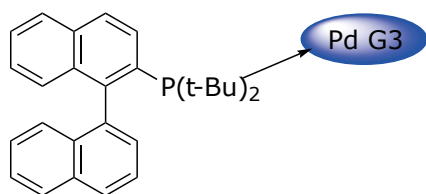
AdBrettPhos Pd G3
MW: 1010.65
100 mg; 500 mg; 2 g; 5 g



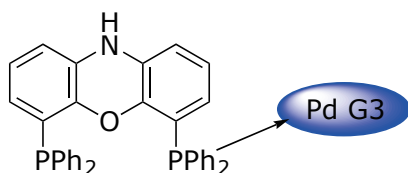
794201

Neopentyl(tBu)₂P Pd G3
MW: 586.08
250 mg; 1 g

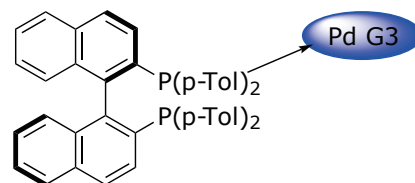
G3 Complexes



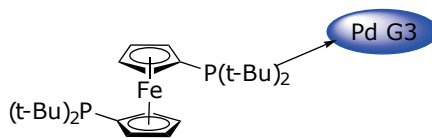
796530
TrixiePhos Pd G3
MW: 768.25
250 mg; 1 g



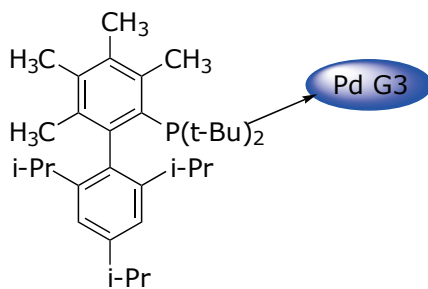
794228
N-XantPhos Pd G3
MW: 921.29
250 mg; 1 g



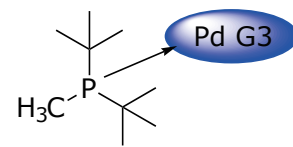
RNI00178
(R)-TolBINAP Pd G3
MW: 1048.51
250 mg



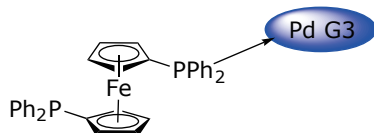
804975*
DTBPF Pd G3
MW: 844.15
250 mg



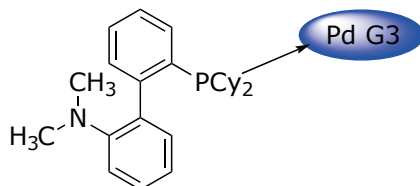
RNI00184
Me₄tBuXPhos Pd G3
MW: 850.48
250 mg



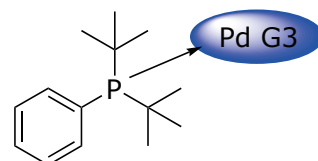
RNI00185
(tBu)₂PMe Pd G3
MW: 529.97
250 mg



804983*
DPPF Pd G3
MW: 954.18
250 mg

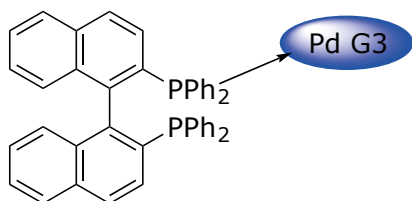


804959*
DavePhos Pd G3
MW: 763.28
250 mg

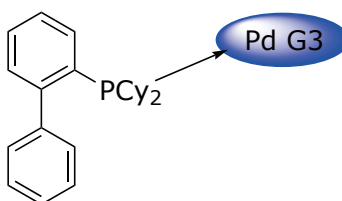


RNI00188
(tBu)₂PPh Pd G3
MW: 592.04
250 mg

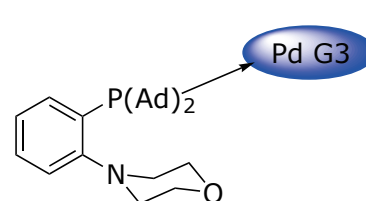
G3 Complexes



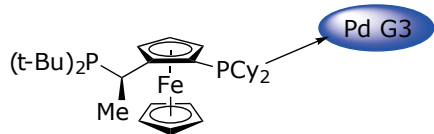
804967*
rac-BINAP Pd G3
MW: 992.40
100 mg



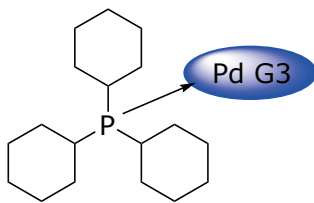
RNI00192
CyJohnPhos Pd G3
MW: 720.21
250 mg



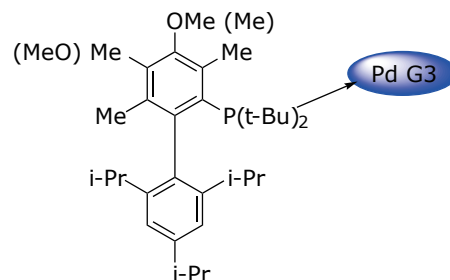
792357
MorDalPhos Pd G3
MW: 833.37
500 mg; 2 g; 5 g



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

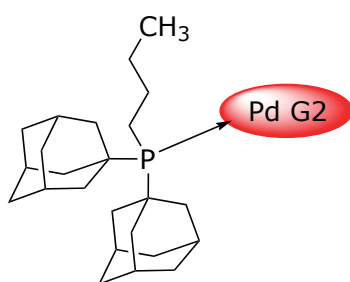
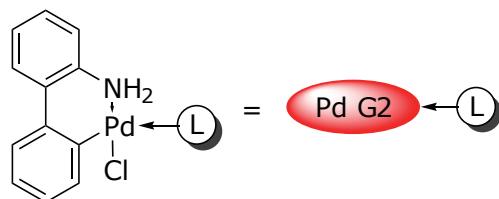


764175
PCy₃ Pd G3
MW: 650.16
250 mg; 1 g; 5 g

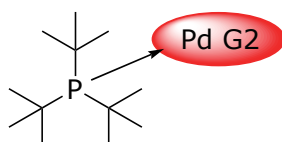


804193*
Me₃(OMe)tBuXPhos Pd G3
MW: 866.49
1 g; 5 g

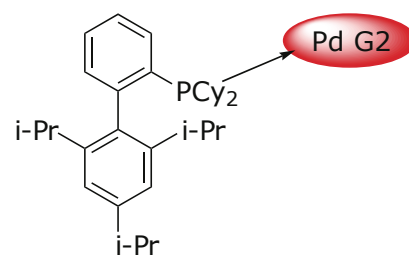
G2 Complexes



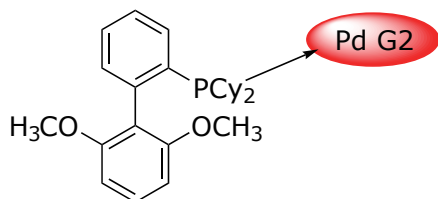
761311
cataCXium A Pd G2
1375477-29-4
MW: 668.63
250 mg; 1 g; 5 g



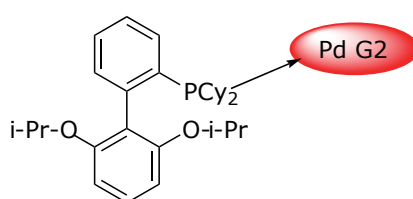
756482
P(t-Bu)₃ Pd G2
1375325-71-5
MW: 512.40
500 mg; 2 g; 5 g



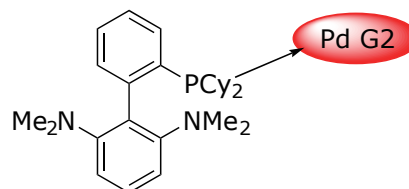
741825
XPhos Pd G2
1310584-14-5
MW: 786.80
250 mg; 1 g; 5 g; 10 g; 25 g; 100 g; 500 g



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

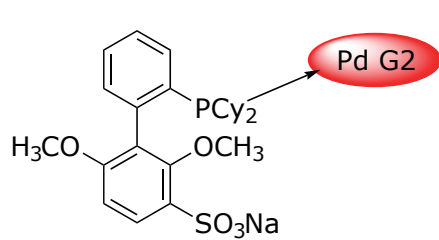


753246
RuPhos Pd G2
1375325-68-0
MW: 776.72
250 mg; 1 g; 5 g

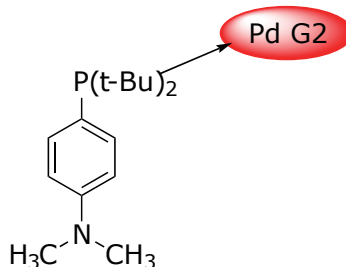


763012
CPhos Pd G2
MW: 746.70
100 mg; 500 mg

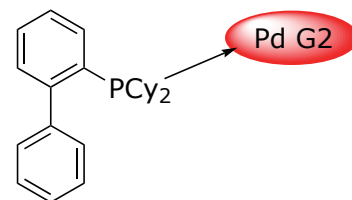
G2 Complexes



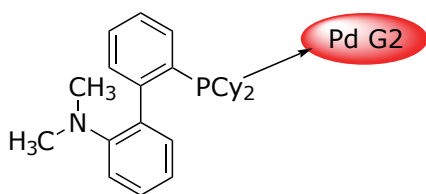
763314
sSPhos Pd G2
(water soluble SPhos)
MW: 822.66
100 mg; 500 mg



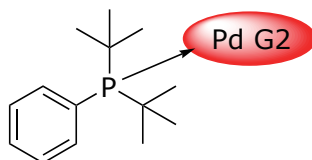
764299
APHos Pd G2
MW: 575.46
500 mg; 2 g



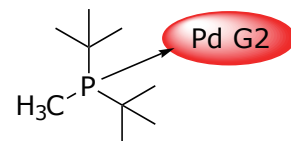
747807
CyJohnPhos Pd G2
MW: 660.56
500 mg; 1 g



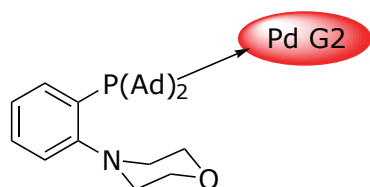
RNI00181
DavePhos Pd G2
MW: 703.63
250 mg



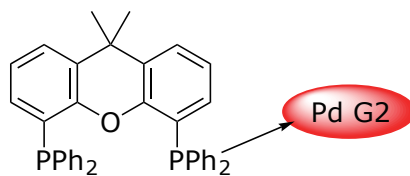
RNI00182
(tBu)₂PPh Pd G2
MW: 532.39
250 mg



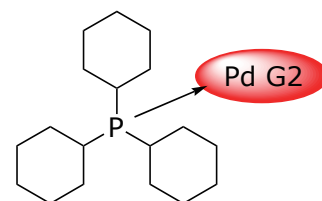
RNI00183
(tBu)₂PMe Pd G2
MW: 470.32
250 mg



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

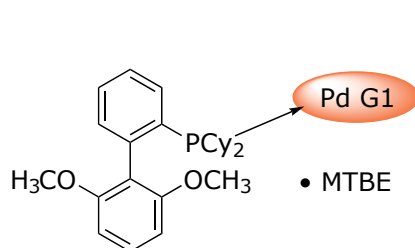
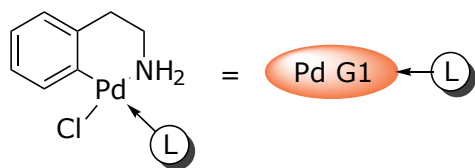


763047
XantPhos Pd G2
1375325-77-1
MW: 888.71
500 mg; 2 g; 5 g

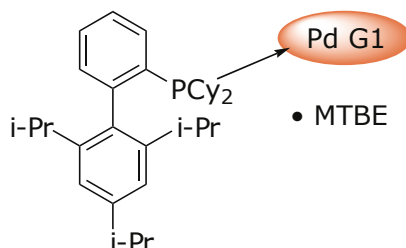


756741
PCy₃ Pd G2
MW: 590.52
1 g; 5 g

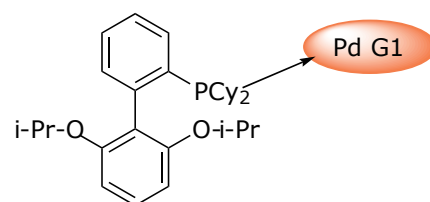
G1 Complexes



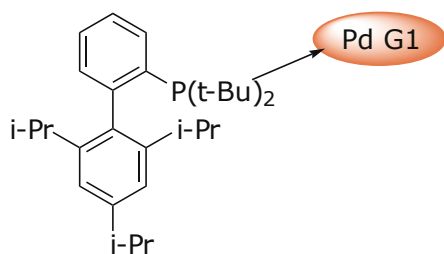
704946
SPhos Pd G1
1028206-58-7
MW: 760.72
250 mg; 1 g



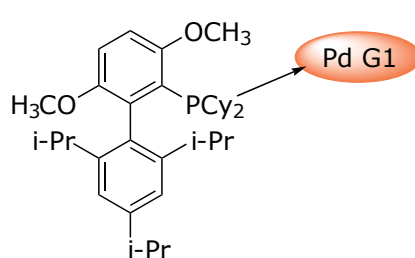
704954
XPhos Pd G1
1028206-56-5
MW: 738.76
250 mg; 1 g



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

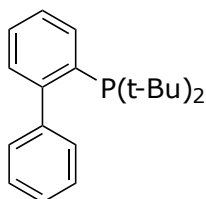


718750
BrettPhos Pd G1
1148148-01-9
MW: 798.81
100 mg; 1 g

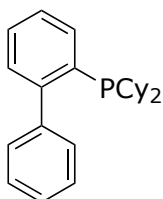


741868
Buchwald Palladacycle Precatalyst Kit
(G1 complexes)
250 mg XPhos, **704954**
250 mg SPhos, **704946**
100 mg RuPhos, **707589**
100 mg tBuXPhos, **708739**
100 mg BrettPhos, **718750**

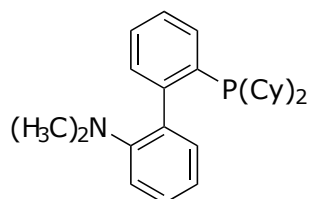
Buchwald Ligands



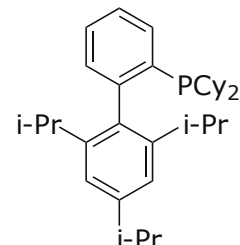
638439
JohnPhos
224311-51-7
MW: 298.40
1 g; 5 g; 25 g; 100 g



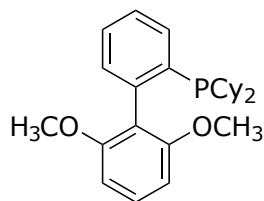
638099
CyJohnPhos
247940-06-3
MW: 350.48
1 g; 5 g; 25 g



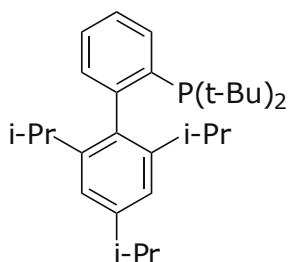
638021
DavePhos
213697-53-1
MW: 393.54
1 g; 5 g; 25 g; 100 g



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



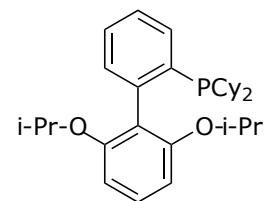
638072
SPhos
657408-07-6
MW: 410.53
1 g; 5 g; 25 g; 500 g



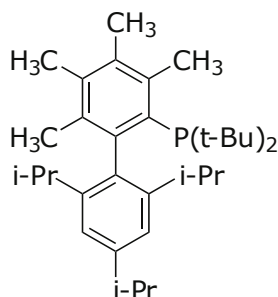
638080
tBuXPhos
564483-19-8
MW: 424.64
1 g; 5 g; 25 g; 100 g; 500 g



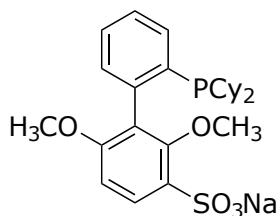
659932
Buchwald Ligands Kit I
1 g JohnPhos, **638439**
1 g CyJohnPhos, **638099**
1 g XPhos, **638064**
1 g tBuXPhos, **638080**
1 g SPhos, **638072**
1 g DavePhos, **638021**



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



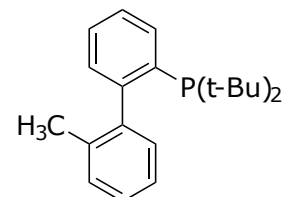
675938
Me.tBuXPhos
857356-94-6
MW: 480.75
250 mg; 1 g; 5 g



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.tBuXPhos, **675938**



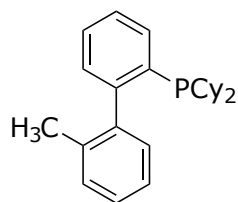
695211
tBuMePhos
255837-19-5
MW: 312.43
1 g

Buchwald Ligands



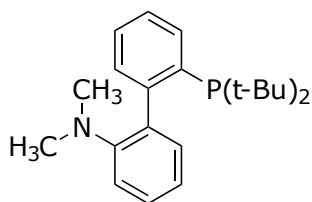
698903

Buchwald Ligands Kit III
 1 g JohnPhos, **638439**
 1 g CyJohnPhos, **638099**
 1 g XPhos, **638064**
 1 g tBuXPhos, **638080**
 1 g SPhos, **638072**
 1 g DavePhos, **638021**
 1 g RuPhos, **663131**
 500 mg sSPhos, **677280**
 250 mg Me₄tBuXPhos, **675938**
 1 g tBuMePhos, **695211**
 1 g MePhos, **695262**
 1 g tBuDavePhos, **695874**
 1 g PhDavePhos, **695882**



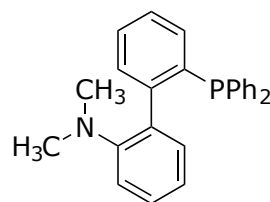
695262

MePhos
 251320-86-2
 MW: 364.50
 1 g; 5 g



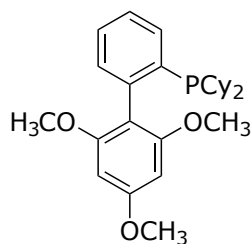
695874

tBuDavePhos
 224311-49-3
 MW: 341.47
 1 g; 5 g



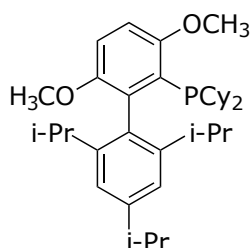
695882

PhDavePhos
 240417-00-9
 MW: 381.45
 1 g; 5 g



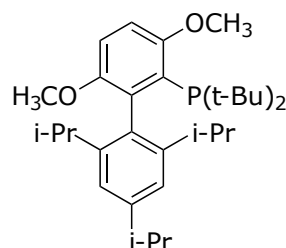
707430

2'-Dicyclohexylphosphino-
 2,4,6-trimethoxybiphenyl
 1000171-05-0
 MW: 440.55
 1 g; 5 g



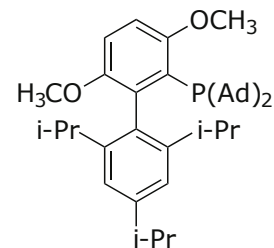
718742

BrettPhos
 1070663-78-3
 MW: 536.77
 100 mg; 500 mg; 1 g; 5 g; 50 g



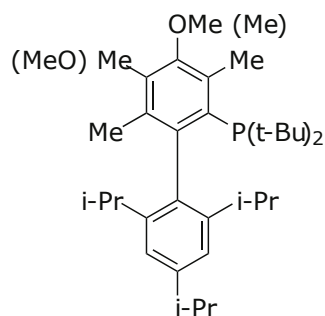
730998

tBuBrettPhos
 1160861-53-9
 MW: 484.69
 100 mg; 500 mg; 5 g; 50 g



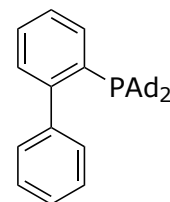
768154

AdBrettPhos
 1160861-59-5
 MW: 640.92
 100 mg; 500 mg; 1 g



792470

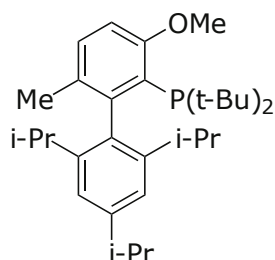
Me₃(OMe)tBuXPhos
 MW: 496.75
 250 mg 1 g; 5 g



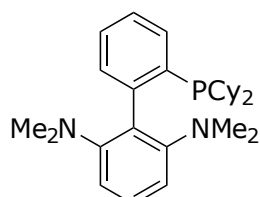
767689

(2-Biphenyl)di-1-adamantylphosphine
 224311-55-1
 MW: 454.63
 250 mg; 1 g

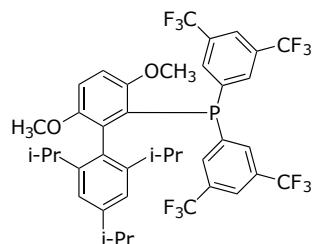
Related Ligands



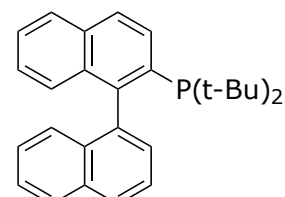
791016
RockPhos
1262046-34-3
MW: 468.69
500 mg; 2 g



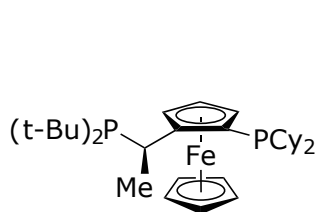
759171
CPhos
1160556-64-8
MW: 436.61
1 g; 5 g



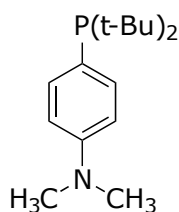
731013
JackiePhos
1160861-60-8
MW: 796.66
100 mg; 250 mg; 1 g



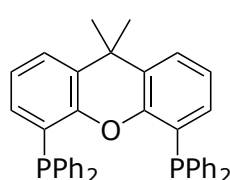
710342
TrixiePhos
255836-67-0
MW: 398.52
500 mg



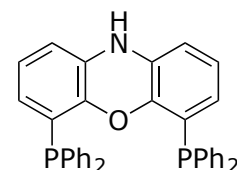
88733
Josephos SL-J009-1
158923-11-6
MW: 554.55
100 mg; 500 mg; 1 g; 5 g



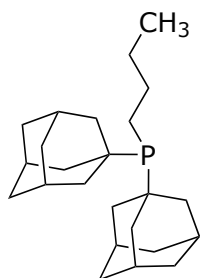
677264
APhos
932710-63-9
MW: 265.37
1 g; 5 g



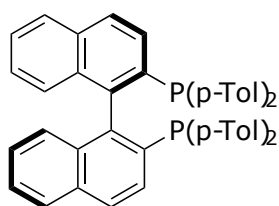
526460
XantPhos
161265-03-8
MW: 578.62
1 g; 5 g; 25 g



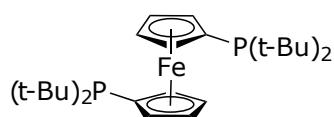
666564
N-XantPhos
(4,6-Bis(diphenylphosphino)
phenoxazine)
261733-18-0
MW: 551.55
500 mg; 1 g



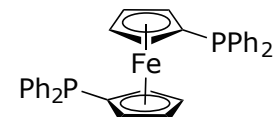
671479
cataCXium A
321921-71-5
MW: 358.54
1 g; 5 g; 50 g; 100 g; 250 g



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

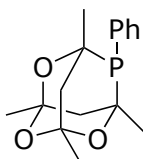


695149
DTBPF
1,1'-Bis(di-tertbutylphosphino)
ferrocene
84680-95-5
MW: 474.42
250 mg; 1 g

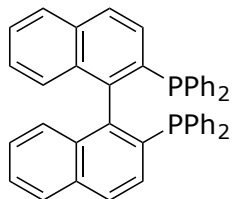


177261
DPPF
1,1'-Bis(diphenylphosphino)
ferrocene
12150-46-8
MW: 554.38
1 g; 10 g; 25 g; 250 g

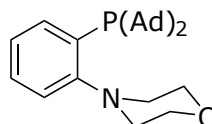
Related Ligands



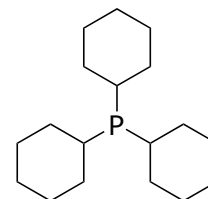
695459
1,3,5,7-Tetramethyl-6-phenyl-2,4,8-trioxa-6-phosphaadamantane
97739-46-3
MW: 292.31
500 mg; 2 g



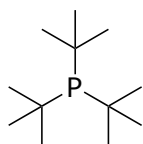
481084
rac-BINAP
2,2'-Bis(diphenylphosphino)-1,1'-binaphthalene
98327-87-8
MW: 622.67
5 g; 25 g; 100 g; 500 g



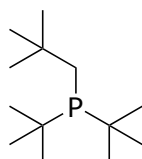
751618
MorDalPhos
Di(1-adamantyl)-2-morpholinophenylphosphine
1237588-12-3
MW: 463.63
250 mg; 1 g



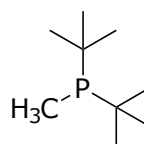
261971
Tricyclohexylphosphine
2622-14-2
MW: 280.43
1 g; 5 g; 25 g; 250 g



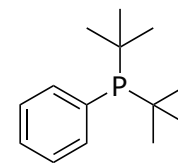
570958
Tri-tert-butylphosphine
13716-12-6
MW: 202.32
1 g; 5 g; 10 g



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	G4 Complex
BrettPhos	718742	718750	—	761605	804355*
AdBrettPhos	768154	—	—	776106	—
tBuBrettPhos	730998	—	—	745979	807877*
DavePhos	638021	—	RNI00181	804959*	—
tBuDavePhos	695874	—	—	—	—
PhDavePhos	695882	—	—	—	—
JohnPhos	638439	—	—	—	—
CyJohnPhos	638099	—	747807	RNI00192	—
MePhos	695262	—	—	—	—
tBuMePhos	695211	—	—	—	—
RuPhos	663131	707589	753246	763403	804290
SPhos	638072	704946	753009	776246	804282
sSPhos	677280	—	763314	—	—
XPhos	638064	704954	741825	763381	804274
tBuXPhos	638080	708739	—	762229	804266*
Me ₃ (OMe)tBuXPhos	792470	—	—	804193*	—
Me ₃ tBuXPhos	675938	—	—	RNI00184	—
(2-Biphenyl)di-1-adamantylphosphine	767689	—	—	—	—
2'-Dicyclohexylphosphino-2,4,6-trimethoxybiphenyl	707430	—	—	—	—
Select Non-Buchwald Ligands					
APhos	677264	—	764299	764183	—
rac-BINAP	481084	—	—	804967*	—
P(t-Bu) ₃	570958	—	756482	—	—
(tBu) ₂ PMe	642629	—	RNI00183	RNI00185	—
(tBu) ₂ PPh	682411	—	RNI00182	RNI00188	—
cataCXium A	671479	—	761311	761435	—
CPhos	759171	—	763012	763004	—
PCy ₃	261971	—	756741	764175	—
DPPF	177261	—	—	804983*	—
DTBPF	695149	—	—	804975*	—
JackiePhos	731013	—	—	762830	—
Josiphos SL-J009-1	88733	—	—	747130	—
MorDalPhos	751618	—	792349	792357	—
Neopentyl(tBu) ₂ P Pd G3	676187	—	—	794201	—
RockPhos	791016	—	—	773905	—
1,3,5,7-Tetramethyl-6-phenyl-2,4,6-trioxa-6-phosphaadamantane	695459	—	—	762822	—
(R)-Tol-BINAP	693049	—	—	RNI00178	—
TrixiePhos	710342	—	—	796530	—
XantPhos	526460	—	763047	763039	—
N-XantPhos	666564	—	—	794228	—

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