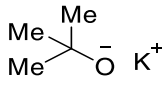
Catalog # 19-1020 CALLERY™ Potassium *tert*-butoxide, 20% solution in tetrahydrofuran

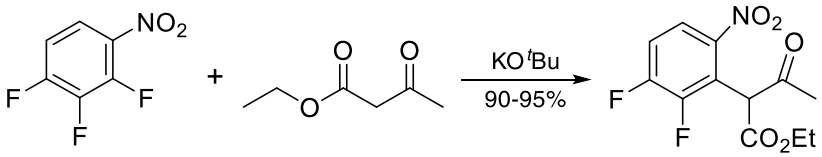


Technical Notes:

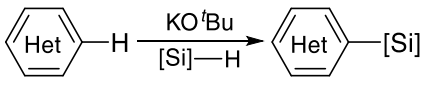
KO^{t}Bu is an essential deprotonating component for numerous organic transformations, acting as a base. Potassium tert-butoxide (also known as potassium tert-butylate, KTB) is quite soluble in ethers and amines but is only slightly soluble in hydrocarbon solvents. The rate of deprotonation with KTB is 5 to 6 orders of magnitude faster than with potassium methoxide. Selective deprotonation can be achieved with KTB due to the steric hindrance provided by the tertiary butyl group.

Transition metal-free application

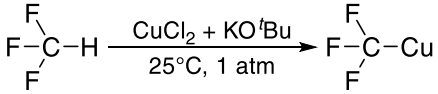
1. **Coupling reactions:** Reagent promoting transition metal-free coupling reactions between ~~KO^{t}Bu~~ KTB and organic additive via direct electron transfer mechanism [1 and references are therein]
2. **Selective Alkylations:** The reaction of trifluoronitrobenzene with a mixture of KTB and ethyl acetoacetate in THF gave >99.9% conversion of desired α-ketoester. The purity of the α-ketoester (75-95%) directly correlated with the level of KOH impurity in KTB.
3. **C–H silylation**: Catalyst for Silylation of C–H bonds in aromatic heterocycles
4. **Cupration**: Used in direct cupration of fluoroform
5. **C–H activation**: Used in graphene oxide co-catalyzed bond activation to generate biaryl compounds in the presence of aryl iodides
6. **Synthesis of carbocycles and heterocycles**: Addition of ketones to acetylenes to generate complex compounds that represent promising synthetic building blocks common in natural products
7. **Synthesis of aryl ethers.** Catalyst for the synthesis of aryl ethers via direct C–O bond formation involving the reaction of alcohols/phenols with aryl ammonium salts, which are easily prepared from anilines
8. **Deuteration:** Catalyst for the α-Selective deuteration of styrene derivatives
9. **C–H Methylation**: Used in C–H methylation of iminoamido heterocycles with sulfur ylides
10. **Elimination reaction**: Used for generation of electron-deficient 1,2-cyclohexadienes via ~~KO^{t}Bu~~ KTB mediated elimination



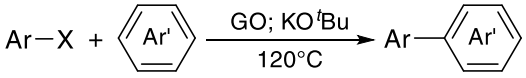
Tech Note (2)
Ref. (2)



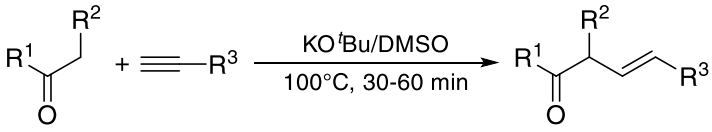
Tech Note (3)
Ref. (3)



Tech Note (4)
Ref. (4)

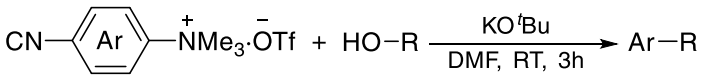


Tech Note (5)
Ref. (5)

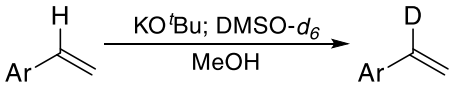


R^1, R^2 = H, alkyl, cycloalkyl, (hetero)aryl; R^3 = (hetero)aryl

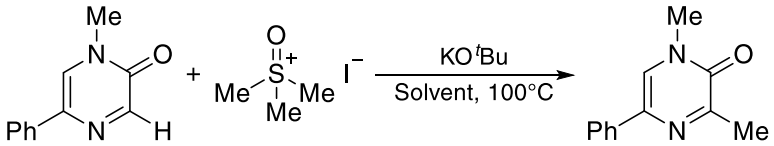
Tech Note (6)
Ref. (6)



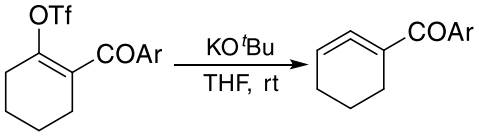
Tech Note (7)
Ref. (7)



Tech Note (8)
Ref. (8)



Tech Note (9)
Ref. (9)



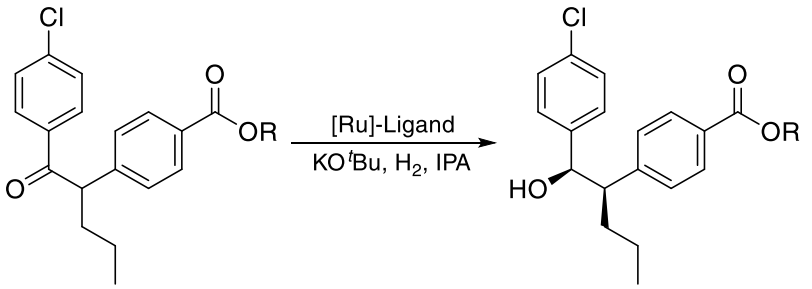
Tech Note (10)
Ref. (10)

References:

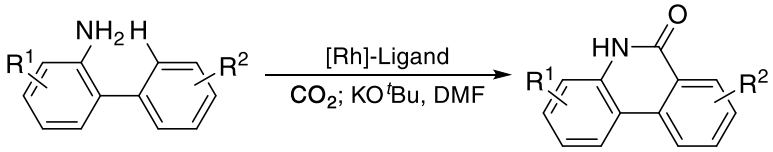
1. *J. Am. Chem. Soc.* **2016**, *138*, 7402
2. *Org. Process Res. Dev.* **2014**, *18*, 89
3. *Nature*, **2015**, *518*, 80
4. *J. Am. Chem. Soc.* **2011**, *133*, 20901
5. *Angew. Chem. Int. Ed.* **2016**, *55*, 3124
6. *Acc. Chem. Res.* **2018**, *51*, 1117
7. *Angew. Chem. Int. Ed.* **2018**, *57*, 3641
8. *J. Am. Chem. Soc.* **2019**, *141*, 1467
9. *Angew. Chem. Int. Ed.* **2021**, *60*, 191
10. *Org. Biomol. Chem.*, **2021**, *19*, 399

Application with transition metals

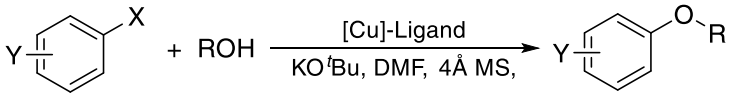
1. **Asymmetric hydrogenation:** Used in the Ru-catalyzed asymmetric hydrogenation via kinetic dynamic resolution of ketone to alcohol
2. **Carboxylation:** Base additive used in the Rh(I)-catalyzed aryl C−H carboxylation of 2-arylanilines with CO_2
3. **Coupling reactions:** Base additive used in the Cu-catalyzed coupling reactions of aryl halides and alcohols to generate alkyl aryl ethers
4. **Carboxylation:** Base additive used in the light/ketone/nickel-catalyzed carboxylation of benzylic and aliphatic C–H bonds with CO_2
5. **Annulation:** Base additive for Ni-catalyzed C−F/N−H annulation of aromatic amides with alkynes
6. **Asymmetric Hydrogenation:** Used in Mn-catalyzed asymmetric hydrogenation of quinolines enabled by π-π interaction
7. **Borylative cyclization:** Base used in enantioselective Cu-catalyzed borylative cyclization for the synthesis of quinazolinones



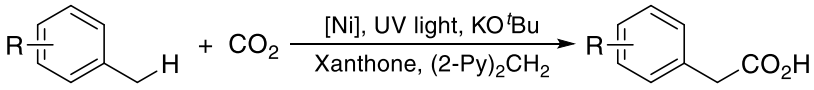
Tech Note (1)
Ref. (1)



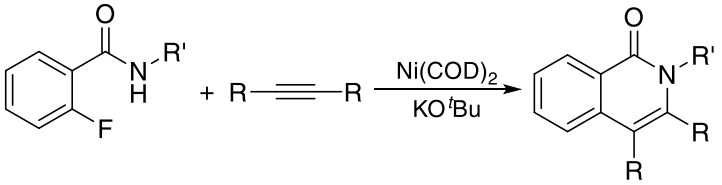
Tech Note (2)
Ref. (2)



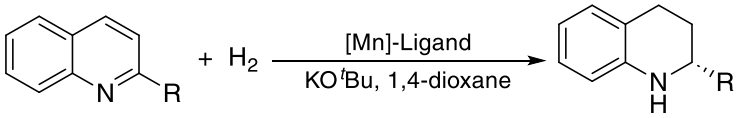
Tech Note (3)
Ref. (3)



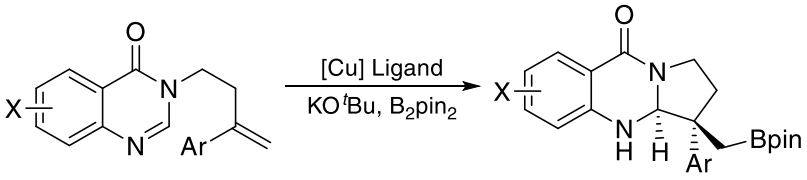
Tech Note (4)
Ref. (4)



Tech Note (5)
Ref. (5)



Tech Note (6)
Ref. (6)



Tech Note (7)
Ref. (7)

References:

1. *Org. Process Res. Dev.* **2012**, *16*, 1832
2. *Org. Lett.* **2019**, *21*, 3663
3. *J. Am. Chem. Soc.* **2019**, *141*, 3541
4. *J. Am. Chem. Soc.* **2019**, *141*, 19611
5. *J. Am. Chem. Soc.* **2020**, *142*, 17306
6. *Angew. Chem. Int. Ed.* **2021**, *60*, 5108
7. *Angew. Chem. Int. Ed.* **2021**, *60*, 14355