

ATH (Asymmetric Transfer Hydrogenation) Catalyst Kit

By using 2-propanol or formic acid as the hydrogen source, asymmetric transfer hydrogenation can avoid the use of high pressure hydrogen gas. In addition, experimental procedures are simple. Ruthenium complexes bearing chiral bidentate nitrogen ligand and arene are highly efficient for reduction of a broad range of ketones and imines to chiral alcohols and amines.

This kit contains 250mg of each of the items listed below. All items are available for individual sale in 250mg, 1g & 5g unit sizes

44-0148 RuCl[(R,R)-Tsdpen](p-cymene)	44-0154 RuCl[(R,R)-Tsdpen](mesitylene)	44-0156 RuCl[(R,R)-Fsdpen](p-cymene)	44-0185 (R,R)-Ts-DENEB®
44-0149 RuCl[(S,S)-Tsdpen](p-cymene)	44-0155 RuCl[(S,S)-Tsdpen](mesitylene)	44-0157 RuCl[(S,S)-Fsdpen](p-cymene)	44-0186 (S,S)-Ts-DENEB®
44-0217 (R)-RUCY®-XylBINAP	44-0218 (S)-RUCY®-XylBINAP	44-0255 Ru-(R,R)-Ms-DENEB®	44-0256 Ru-(S,S)-Ms-DENEB®

96-6955 Takasago ATH (Asymmetric Transfer Hydrogenation) Catalyst

Item#	Acronym	CAS#	Item#	Acronym	CAS#
44-0148	RuCl[(R,R)-Tsdpen](p-cymene)	192139-92-7	44-0149	RuCl[(S,S)-Tsdpen](p-cymene)	192139-90-5
44-0154	RuCl[(R,R)-Tsdpen](mesitylene)	174813-82-2	44-0155	RuCl[(S,S)-Tsdpen](mesitylene)	174813-81-1
44-0156	RuCl[(R,R)-Fsdpen](p-cymene)	1026995-71-0	44-0157	RuCl[(S,S)-Fsdpen](p-cymene)	1026995-72-1
44-0185	(R,R)-Ts-DENEB®	1333981-84-2	44-0186	(S,S)-Ts-DENEB®	1384974-37-1
44-0217	(R)-RUCY XylBINAP	1384974-38-2	44-0218	(S)-RUCY XylBINAP	1312713-89-5
44-0255	(R,R)-Ms-DENEB®	1333981-86-4	44-0256	(S,S)-Ms-DENEB®	1361318-83-3

Sold in collaboration with Takasago

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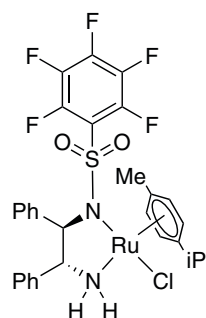
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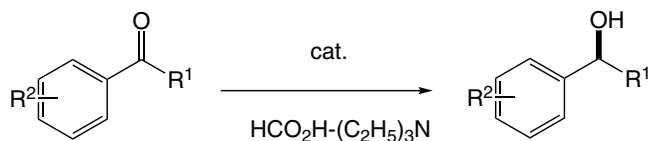
44-0156 Chloro[[**(1R,2R)**-(-)-2-amino-1,2-diphenylethyl](pentafluorophenylsulfonyl)amido}(p-cymene)ruthenium(II), min. 90% RuCl[(R,R)-Fsdpen](p-cymene) (1026995-71-0)
 C₃₀H₂₈ClF₅N₂O₂RuS; FW: 712.14; orange to brown powdr.
air sensitive
 Note: Sold in collaboration with Takasago.

250mg
1g
5g



Technical Note:

1. Catalyst used in the asymmetric transfer hydrogenation of ketones using formic acid-triethylamine mixture.



Tech. Note (1)
Ref. (1)

References:

1. *J. Am. Chem. Soc.*, **1996**, *118*, 2521.

44-0157 Chloro[[**(1S,2S)**-(+)-2-amino-1,2-diphenylethyl](pentafluorophenylsulfonyl)amido}(p-cymene)ruthenium(II), min. 90% RuCl[(S,S)-Fsdpen](p-cymene) (1026995-72-1)
 C₃₀H₂₈ClF₅N₂O₂RuS; FW: 712.14; orange to brown powdr.
air sensitive
 Note: Sold in collaboration with Takasago. Takasago ATH Catalyst Kit component.

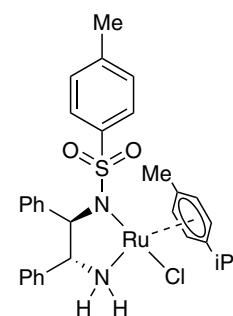
250mg
1g
5g

44-0149 Chloro[[**(1S,2S)**-(+)-2-amino-1,2-diphenylethyl](4-toluenesulfonyl)amido}(p-cymene)ruthenium(II), min. 90% RuCl[(S,S)-Tsdpen](p-cymene) (192139-90-5)
 C₃₁H₃₅ClN₂O₂RuS; FW: 636.21; yellow to dark brown solid
air sensitive
 Note: Sold in collaboration with Takasago. Takasago ATH Catalyst Kit component.

250mg
1g
5g

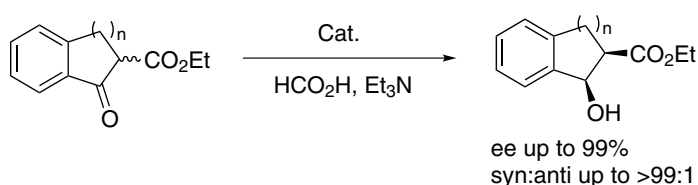
44-0148 Chloro[[**(1R,2R)**-(-)-2-amino-1,2-diphenylethyl](4-toluenesulfonyl)amido}(p-cymene)ruthenium(II), min. 95% RuCl[(R,R)-Tsdpen](p-cymene) (192139-92-7)
 C₃₁H₃₅ClN₂O₂RuS; FW: 636.21; yellow to dark brown solid
air sensitive
 Note: Sold in collaboration with Takasago. Takasago ATH Catalyst Kit component.

250mg
1g
5g

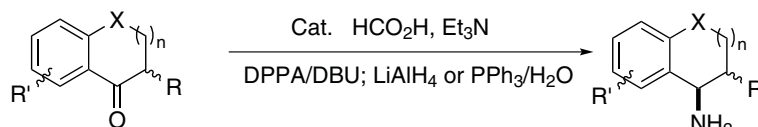


Technical Note:

1. This catalyst has shown to effect highly enantioselective hydrogenation of functionalized ketones where the substituents are dialkylamino, hydroxy, siloxy, carbonyl, ester, amide or thioester.



Tech. Note (1)
Ref. (1)



Tech. Note (1)
Ref. (2)

n = 0, 1; R = alkyl, F, OAc; X = CH₂, O

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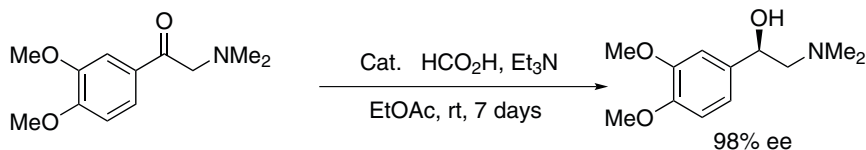
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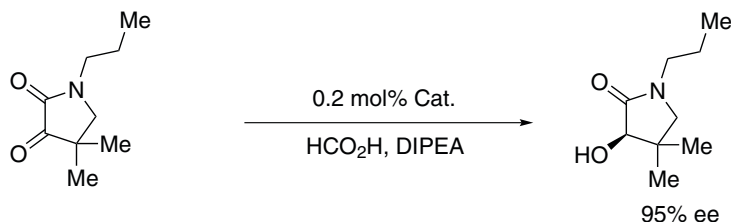
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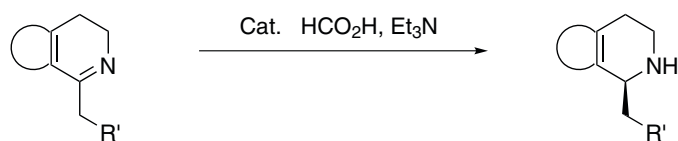
44-0148 Chloro{[(1R,2R)-(-)-2-amino-1,2-diphenylethyl](4-toluenesulfonylamido)}(p-cymene)ruthenium(II), min. 95%
(continued) RuCl[(R,R)-Tsdpen](p-cymene) (192139-92-7)



Tech. Note (1)
Ref. (3)



Tech. Note (1)
Ref. (4-6)



Tech. Note (1)
Ref. (7,8)

References:

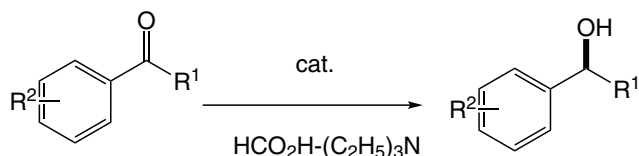
1. *Tetrahedron*, **2007**, 63, 7532
2. *Tetrahedron*, **2007**, 63, 6755
3. *Tetrahedron: Asymmetry*, **2009**, 20, 1138
4. *J. Org. Chem.*, **2009**, 74, 1411
5. *Org. Lett.*, **2007**, 9, 2461
6. *Org. Lett.*, **2009**, 11, 935
7. *Angew. Chem. Int. Ed.*, **2009**, 48, 7616
8. *Bioorg. Med. Chem. Lett.*, **2008**, 18, 4110

44-0154 Chloro{[(1R,2R)-(-)-2-amino-1,2-diphenylethyl](4-toluenesulfonylamido)}
(mesitylene)ruthenium(II), min. 90% RuCl[(R,R)-Tsdpen(mesitylene) (174813-82-2)
C₃₀H₃₃ClN₂O₂RuS; FW: 622.18; orange powdr.
air sensitive

Note: Sold in collaboration with Takasago. Takasago ATH Catalyst Kit component.

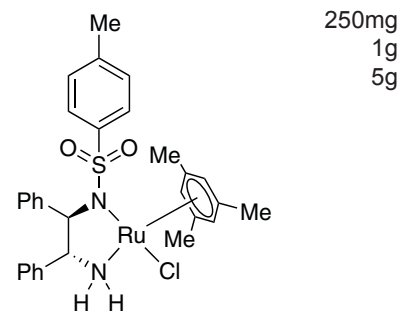
Technical Note:

1. Catalyst used in the asymmetric transfer hydrogenation of ketones using formic acid-triethylamine mixture.



References:

1. *J. Am. Chem. Soc.*, **1996**, 118, 2521.



Tech. Note (1)
Ref. (1)

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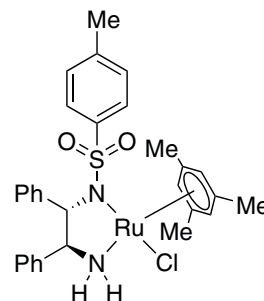
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44-0155 Chloro{[(1S,2S)-(+)-2-amino-1,2-diphenylethyl](4-toluenesulfonylamido) (mesitylene)ruthenium(II), min. 90% RuCl[(S,S)-Tsdpen](mesitylene) (174813-81-1)
 $C_{30}H_{33}ClN_2O_2RuS$; FW: 622.18; yellow to dark brown solid
air sensitive
 Note: Sold in collaboration with Takasago. US7129367B2. Takasago ATH Catalyst Kit component.

250mg
1g
5g

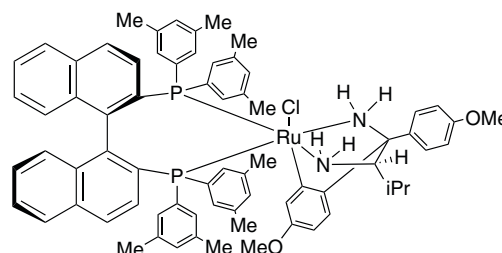


Technical Note:

- See 44-0154 (page 3)

44-0217 Chloro{(R)-(+)-2,2'-bis[di(3,5-xylyl)phosphino]-1,1'-binaphthyl} [(2R)-(-)-1-(4-methoxyphenyl)-1'-(4-methoxyphenyl)-kC]-3-methyl-1,2-butanediamine]ruthenium(II) (R)-RUCY®XylBINAP (1384974-38-2)
 $C_{71}H_{73}ClN_2O_2P_2Ru$; FW: 1184.82;
 yellow to dark brown/green solid
air sensitive
 Note: Sold in collaboration with Takasago. US Patent 9079931. Takasago BINAP Ru Diamine Catalyst Kit component. Takasago ATH Catalyst Kit component.

100mg
250mg
1g
5g

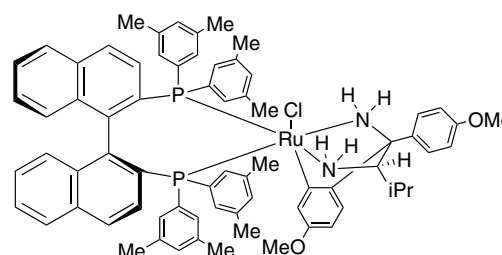


Technical Note:

- See 44-0218 (page 4)

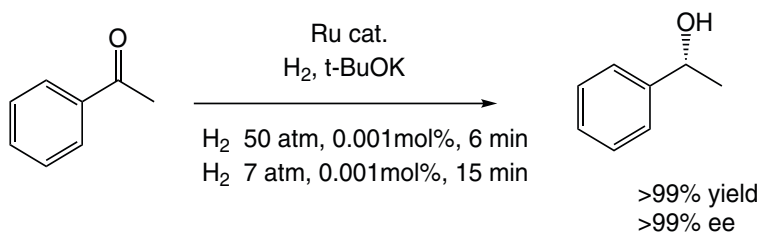
44-0218 Chloro{(S)-(-)-2,2'-bis[di(3,5-xylyl) phosphino]-1,1'-binaphthyl}[(2S)- (+)-1-(4-methoxyphenyl)-1'-(4-methoxyphenyl)-kC]-3-methyl-1,2-butanediamine]ruthenium(II) (S)-RUCY®XylBINAP (1312713-89-5)
 $C_{71}H_{73}ClN_2O_2P_2Ru$; FW: 1184.82;
 yellow to dark brown/green solid
air sensitive
 Note: Sold in collaboration with Takasago. US Patent 9079931. Takasago BINAP Ru Diamine Catalyst Kit component. Takasago ATH Catalyst Kit component.

250mg
1g
5g



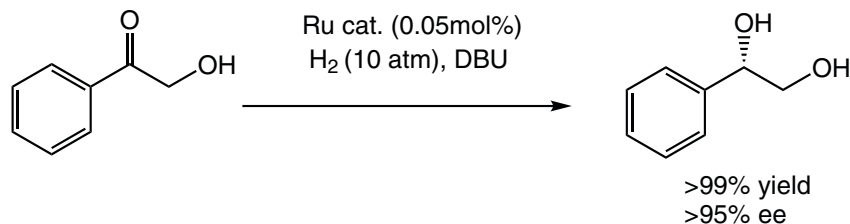
Technical Note:

- Catalyst used for the rapid, and highly selective hydrogenation of ketones.



Tech. Note (1)
Ref. (1)

"trans-RuCl₂(xylbinap)(daipen) 0.001 mol%, 240 min"



Tech. Note (1)
Ref. (1)

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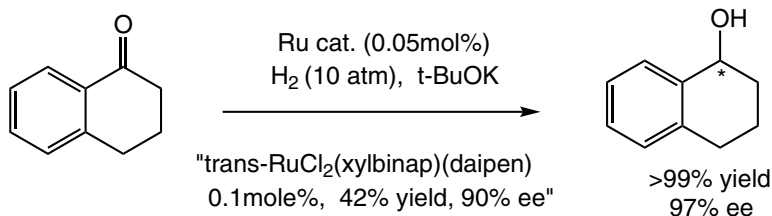
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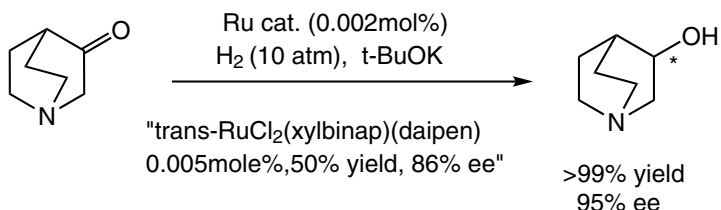
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44-0218 Chloro{(S)-(-)-2,2'-bis[di(3,5-xylyl) phosphino]-1,1'-binaphthyl}[(2S)-(+)-1-(4-methoxyphenyl)-1'-(4-methoxyphenyl)-kC]-3-methyl-1,2-butanediamine]ruthenium(II) (S)-RUCY®XylBINAP (1312713-89-5)
(continued)



Tech. Note (1)
Ref. (1)

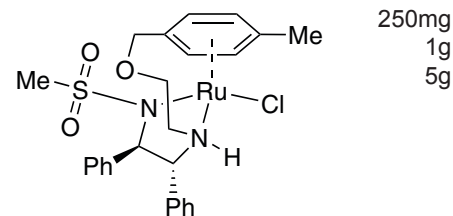


Tech. Note (1)
Ref. (1)

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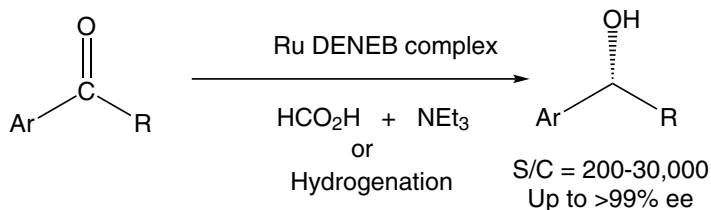
- (a) US. Pat. 9079931. (b) *J. Am. Chem. Soc.*, 2011, 133, 10696.

44-0255 Chloro{N-[(1R,2R)-2-[(S)-[2-[[1,2,3,4,5,6-η]-4-methylphenyl]methoxy]ethyl]amino]-1,2-diphenylethylmethanesulfonamidato}ruthenium(II) (R,R)-Ms-DENE^B® (1333981-86-4)
C₂₅H₂₉ClN₂O₃RuS; FW: 574.10; light to dark brown powdr.
Note: Sold in collaboration with Takasago. US. Patent 9217005.
Takasago ATH Catalyst Kit component.

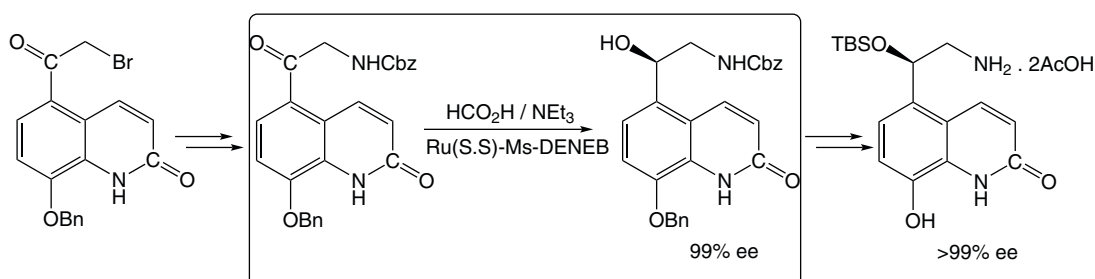


Technical Notes:

- Catalyst used for both hydrogenation and asymmetric transfer hydrogenation.
- Ruthenium catalyst used as a key intermediate in a synthesis of a receptor agonist.



Tech. Note (1)
Ref. (1)



Tech. Note (2)
Ref. (2)

References:

- J. Am. Chem. Soc.*, 2011, 133, 14960
- Org. Process Res. Dev.*, 2015, 19, 315

44-0256 Chloro{N-[(1S,2S)-2-[(R)-[2-[[1,2,3,4,5,6-η]-4-methylphenyl]methoxy]ethyl]amino]-1,2-diphenylethylmethanesulfonamidato}ruthenium(II) (S,S)-Ms-DENE^B® (1361318-83-3)
C₂₅H₂₉ClN₂O₃RuS; FW: 574.10; light to dark brown powdr.
Note: Sold in collaboration with Takasago. US. Patent 9217005. Takasago ATH Catalyst Kit component.

250mg
1g
5g

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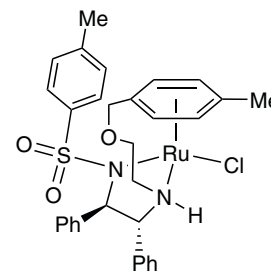
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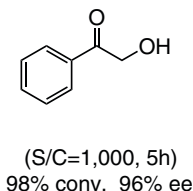
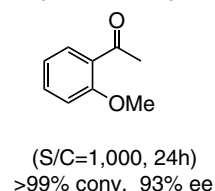
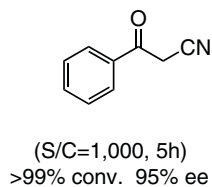
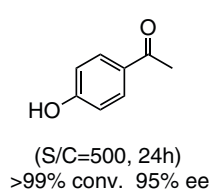
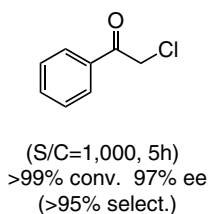
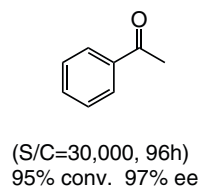
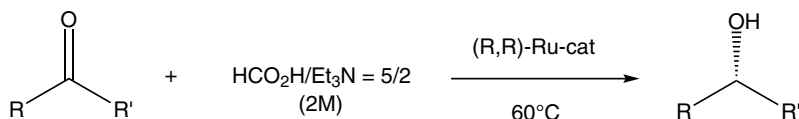
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 (1333981-84-2)
 C₃₁H₃₃ClN₂O₃RuS; FW: 650.19; gray to brown solid
 Note: Sold in collaboration with Takasago. US. Patent 9079931.

250mg
 1g
 5g

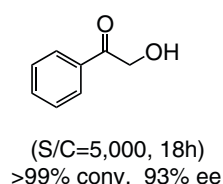
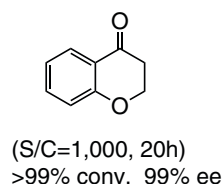
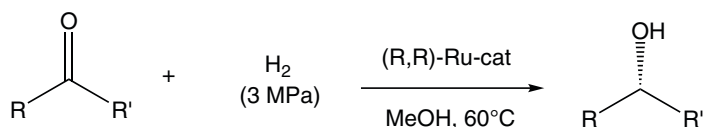


Technical Notes:

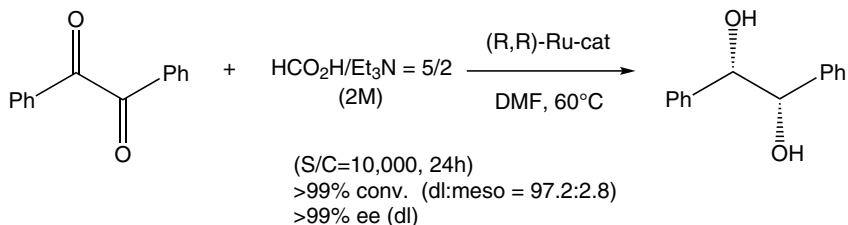
1. Catalyst used for asymmetric α -transfer hydrogenation.
2. Catalyst used for asymmetric H₂ – hydrogenation.
3. Catalyst used for dynamic kinetic resolution.
4. Catalyst used for asymmetric transfer hydrogenation of unsymmetrical benzophenones.
5. Catalyst used for asymmetric transfer hydrogenation of Aryl N-Heteroaryl Ketones.
6. Catalyst used for asymmetric transfer hydrogenation of alpha-Substituted Ketone.



Tech. Note (1)
 Ref. (1)



Tech. Note (2)
 Ref. (1)



Tech. Note (3)
 Ref. (1)

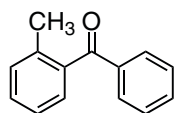
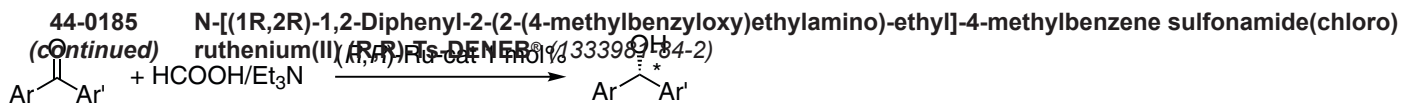
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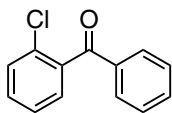
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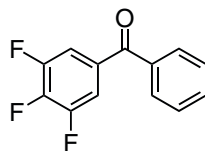
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(60 °C, 18 h)
98% yield. 98% ee

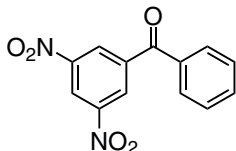


(40 °C, 17 h)
>99% yield. 98% ee

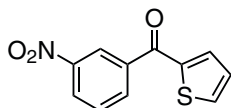


(30 °C, 16 h)
>99% yield. 95% ee

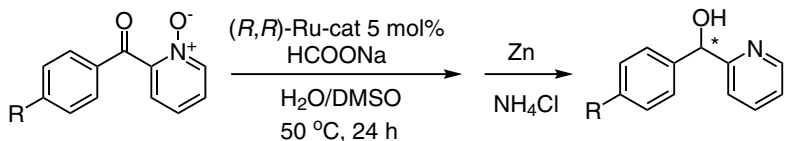
Tech. Note (4)
Ref. (2)



(30 °C, 26 h)
90% yield. >99% ee

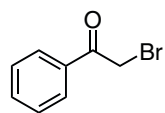
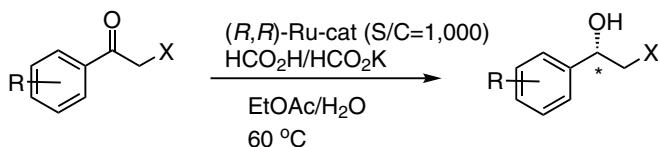


(10 °C, 8 h)
96% yield. 98% ee

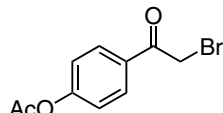


R=H : 86% yield. 97.8% ee
R=Cl : 92% yield. 99.8% ee

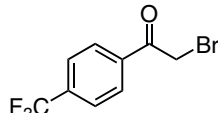
Tech. Note (5)
Ref. (3)



(4 h)
93% yield. 96% ee



(6 h)
93% yield. 95% ee



(4 h)
94% yield. 94% ee

Tech. Note (6)
Ref. (4)

References:

1. *J. Am. Chem. Soc.*, **2011**, *133*, 14960
2. *J. Am. Chem. Soc.* **2016**, *138*, 10084.
3. *Org. Lett.* **2017**, *19*, 2094.
4. *Adv. Synth. Catal.* **2017**, *360*, 568

44-0186 N-[(1*S*,2*S*)-1,2-Diphenyl-2-(2-(4-methylbenzyloxy)ethylamino)-ethyl]-4-methylbenzene sulfonamide(chloro) 250mg
ruthenium(II) (**S,S**)-Ts-DENE^B® (1384974-37-1) 1g
C₃₁H₃₃ClN₂O₃RuS; FW: 650.19; gray to brown solid 5g
Note: Sold in collaboration with Takasago. US Pat. 9217005, US Pat. 9073827.

Technical Note:

1. See 44-0185 (page 6)

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