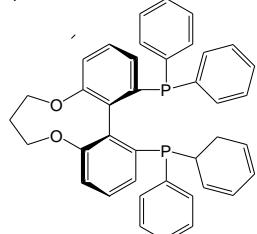


# Catalyst and Ligand Toolbox Kit for Asymmetric Hydrogenation

Kit# 96-5900

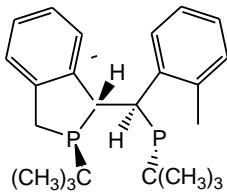
Contains 100mg of each of the items listed below.

Cat. # 15-0175 (R)-C<sub>3</sub>-TUNEPHOS

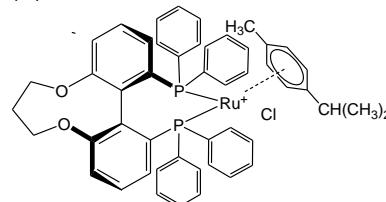


Cat. # 15-0176 (S)-C<sub>3</sub>-TUNEPHOS

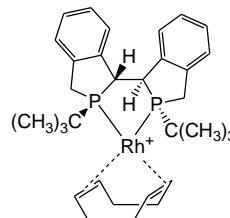
Cat. # 15-1060 (R,R,S,S)-DUANPHOS



Cat. # 44-0109 (R)-C<sub>3</sub>-TUNEPHOS-Ru



Cat. # 45-0663 (R,R,S,S)-DUANPHOS-Rh



Available in 100mg and 500mg standard sizes.

**15-0175 R-(*-*)-1,13-Bis(diphenylphosphino)-7,8-dihydro-6H-dibenzo[*f,h*][1,5]dioxonin, 97% (R)-C<sub>3</sub>-TUNEPHOS**  
[301847-89-2] C<sub>39</sub>H<sub>32</sub>O<sub>2</sub>P<sub>2</sub>; FW: 594.62; white pwdr.

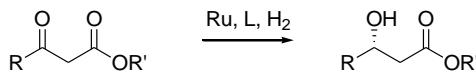
100mg  
500mg

*air sensitive*

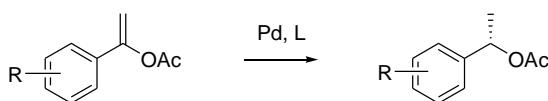
Note: US Patent No. 6,521,769; additional patents pending.

#### Technical Notes:

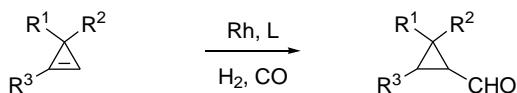
1. New generation of chiral biaryl phosphine ligands with tunable dihedral angles. The ability to modify the dihedral angle allows for the fine tuning of the catalyst system and optimization of enantioselectivity.
2. Ru-C<sub>3</sub>-TUNEPHOS complexes are used for asymmetric hydrogenation of β-ketoesters<sup>1</sup>, enol acetates<sup>2</sup>, cyclic β-amino acids<sup>3</sup>, α-phthalimide ketones<sup>4</sup>, and α-keto esters<sup>5</sup>.
3. Rh-catalyzed hydroformylation of cyclopropenes.



Tech. Note (2)  
Ref. (1)



Tech. Note (2)  
Ref. (2)



Tech. Note (3)  
Ref. (6)

#### References:

1. *J. Org. Chem.*, **2000**, 65, 6223.
2. *Org. Lett.*, **2002**, 4, 4495.
3. *J. Am. Chem. Soc.*, **2003**, 125, 9570.
4. *J. Am. Chem. Soc.*, **2004**, 126, 1626.
5. *Synlett*, **2006**, 126, 1169.
6. *J. Am. Chem. Soc.*, **2008**, 130, 13804.

|         |   |                |
|---------|---|----------------|
| 15-0176 | <b>(S)-(+)-1,13-Bis(diphenylphosphino)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin, 95% (S)-C<sub>3</sub>-TUNEPHOS</b><br>[486429-99-6] C <sub>39</sub> H <sub>32</sub> O <sub>2</sub> P <sub>2</sub> ; FW: 594.62; white pwdr.<br>air sensitive | 100mg<br>500mg |
|---------|---|----------------|

Note: US Patent No. 6,521,769; additional patents pending.

Technical Note:

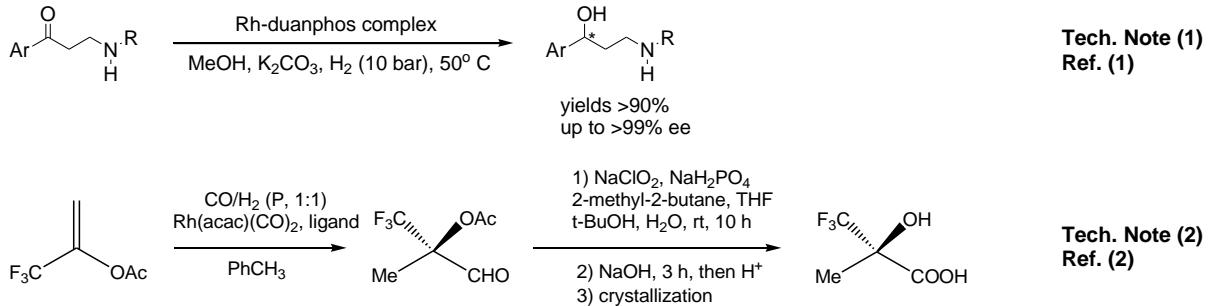
- See 15-0175.

|         |   |                |
|---------|---|----------------|
| 15-1060 | <b>(1R,1'R,2S,2'S)-(+)-2,2'-Di-t-butyl-2,3,2',3'-tetrahydro-1,1'-bi-1H-isophosphindole, min. 98% (R,R,S,S)-DUANPHOS</b><br>[528814-26-8] C <sub>24</sub> H <sub>32</sub> P <sub>2</sub> ; FW: 382.46; white xtl.; [α] <sub>D</sub> +19.5<br>air sensitive | 100mg<br>500mg |
|---------|---|----------------|

Note: Patent pending, PCT/US02/35788.

Technical Notes:

- As a highly electron-donating and conformationally rigid ligand, the rhodium complex of DuanPhos has exhibited remarkably high enantioselectivities and reactivities for the hydrogenation of a variety of functionalized olefins.
- Rhodium/DUANPHOS catalyst used in the synthesis of 2-trifluoromethyl lactic acid by asymmetric hydroformylation.



References:

- Angew. Chem. Int. Ed., 2005, 44, 1687.
- J. Org. Chem., 2013, 78, 3429.

|         |   |                |
|---------|---|----------------|
| 45-0663 | <b>(1R,1'R,2S,2'S)-(+)-2,2'-Di-t-butyl-2,3,2',3'-tetrahydro-1,1'-bi-1H-isophosphindole(1,5-cyclooctadiene)rhodium(I) tetrafluoroborate, min. 98% (R,R,S,S)-DUANPHOS-Rh</b><br>[Rh(C <sub>8</sub> H <sub>12</sub> )(C <sub>24</sub> H <sub>32</sub> P <sub>2</sub> )] <sup>+</sup> BF <sub>4</sub> <sup>-</sup> ; FW: 680.35; orange xtl.<br>air sensitive | 100mg<br>500mg |
|---------|---|----------------|

Note: US Patent No. 7105702, 7153809, 7169953.

Technical Note:

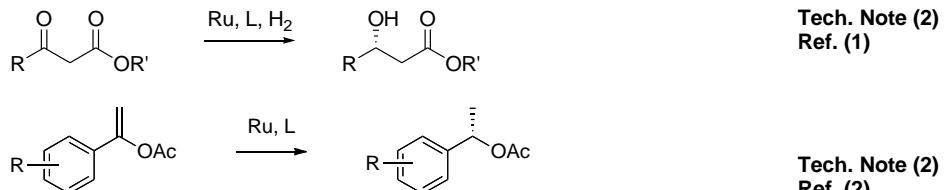
- See 15-1060.

|         |   |                |
|---------|---|----------------|
| 44-0109 | <b>Chloro((R)-(-)-1,13-bis(diphenylphosphino)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin)(p-cymene)ruthenium(II) chloride (R)-C<sub>3</sub>-TUNEPHOS-Ru</b><br>[RuCl(C <sub>39</sub> H <sub>32</sub> O <sub>2</sub> P <sub>2</sub> )(C <sub>10</sub> H <sub>14</sub> )] <sup>+</sup> Cl <sup>-</sup> ; FW: 900.81; orange to brown pwdr.<br>air sensitive | 100mg<br>500mg |
|---------|---|----------------|

Note: Patent US 6,521,769.

Technical Notes:

- New generation of chiral biaryl phosphine ligands with tunable dihedral angles. The ability to modify the dihedral angle allows for the fine tuning of the catalyst system and optimization of enantioselectivity. See 15-0175 (page !\_!blue15-0175!\_!).
- Ru-C<sub>3</sub>-TUNEPHOS complexes are used for asymmetric hydrogenation of β-ketoesters<sup>1</sup>, enol acetates<sup>2</sup>, cyclic β-amino acids<sup>3</sup>, α-phthalimide ketones<sup>4</sup>, and α-keto esters<sup>5</sup>.



References:

- J. Org. Chem., 2000, 65, 6223.
- Org. Lett., 2002, 4, 4495.
- J. Am. Chem. Soc., 2003, 125, 9570.
- J. Am. Chem. Soc., 2004, 126, 1626.
- Synlett., 2006, 126, 1169.