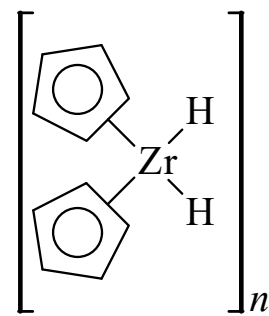




>>Entry Name: Bis(η^5 -2,4-cyclopentadien-1-yl)dihydrozirconium, 10CI

Synonym(s): Zirconocene dihydride



CAS Registry Number: 37342-98-6

Molecular Formula: C₁₀H₁₂Zr

Molecular Weight: 223.429

Accurate Mass: 221.998603

Percentage Composition: C 53.76%; H 5.41%; Zr 40.83%

General Statement: Polymeric

Source/Synthesis: Synth. from ZrCp₂Me₂ and H₂ at 60 atm. and 80°

Use/Importance: Hydrogenation catalyst for alkenes and alkynes. With 2-propanol, catalyses 1,2-redn. of α,β - unsatd. carbonyls to allylic alcohols and redn. of quinone to 1, 4-dihydroxybenzene; reduces ketones; dimerises aldehydes to esters under mild conditions; catalyses Meerwein Ponderff-Verley redn.; undergoes stoichiometric hydrometallation of alkenes; catalyses Oppenauer oxidn.; catalyses chemoselective redn. of polycarbonyls to hydroxycarbonyls; catalyses the redn. of β -hydroxy ketones by aldehydes giving diol monoesters with high stereoselectivity; catalyses the redn. of β hydroxy ketones by aldehydes giving diol monoesters with high stereoselectivity

Physical Description: Colourless microcryst.

Solubility: Insol. common solvs.

References:

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Wales, P.C. *et al.*, *J. Organomet. Chem.*, 1971, **27**, 373; 1972, **43**, C29, (*use, hydrometallation, ir*)
Weil, P.A. *et al.*, *J. Organomet. Chem.*, 1973, **49**, 227, (*use, hydrogenation*)
Labinger, J.A. *et al.*, *J. Organomet. Chem.*, 1978, **155**, C25, (*use, redn of ketones*)
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Ishii, Y. *et al.*, *J.O.C.*, 1986, **51**, 240, (*use, oxidn*)
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Umekawa, Y. *et al.*, *J.O.C.*, 1997, **62**, 3409-3412, (*use, redn of β -hydroxyketones*)
Umekawa, Y. *et al.*, *J.O.C.*, 1997, **62**, 3409-3412, (*use, redn of β -hydroxyketones*)