



>>Entry Name: Dichlorobis(η^5 -2,4-cyclopentadien-1-yl)titanium, 9Cl

Synonym(s): Bis(cyclopentadienyl)titanium dichloride. Titanocene dichloride

CAS Registry Number: 1271-19-8

BB0266 BB0300 BB0330 BB0370 BB0380 BB0670 BB0400 BB0480 BB0650

As Dibromobis(η^5 -2,4-cyclopentadien-1-yl)titanium, BQF36-E with
X = Cl

Molecular Formula: C₁₀H₁₀Cl₂Ti

Molecular Weight: 248.974

Accurate Mass: 247.963901

Percentage Composition: C 48.24%; H 4.05%; Cl 28.48%; Ti 19.23%

Source/Synthesis: Synth. from TiCl₄ and NaCp or CpMgCl

Use/Importance: Reagent for formn. of Ti enolates. Catalyst for: hydromagnesiation of alkynes (e.g. by BuⁱMgBr), alkenes, allyl or homoallyl alcohols, propargyl alcohols; hydroalumination of alkynes, alkenes, dienes; carbometallation of alkynes, alkynylsilanes; carbomagnesiation of isoprene; redn. of carboxylic acids (but not α,β -unsatd. acids) with BuⁱMgBr $\rightarrow$ aldehydes; redn. of aliphatic aldehydes, ketones with BuⁱMgX, H₃CCH₂CH₂MgX, PrⁱMgX; redn. of vinyl, aryl, alkyl bromides with PrⁱMgBr; redn. of R₃SiOR' $\rightarrow$ R₃SiH; redn. of aromatic aldehydes with Bu^sMgCl $\rightarrow$ pinacols with high *syn*-stereoselection; with LiAlH₄, reagent for inter- and intramolecular reductive coupling of aldehydes, ketones $\rightarrow$ pinacols; with Bu^sMgCl, effects highly *lk*-selective hydrodimerisation of α,β -unsatd. aldehydes; catalyses hydroboration of alkenes, dienes, alkynes using NaBH₄, LiBH₄; hydrogenation of vinyl esters, unsatd. polymers with BuLi; hydrogenolysis of allylic alcohols by LiAlH₄ and of RBr by PrⁱMgCl; with MePPh₂ and Na/Hg, effects intramolecular cyclisation of diynes to give, after hydrol., 5-, 6- or 7-membered rings with an (*E,E*)-exocyclic diene; *in situ* redn. with Zn gives Cp₂TiCl which effects debromination of *vic*-dibromides to alkenes by *anti*-elimination; with AlMe₃, reagent for methylenation of ketones, esters and with R₃Al substitutes 1-alkenes $\rightarrow$ RR'C=CH₂; with Mg, deoxygenates epoxides; with alkyl Al complexes, Ziegler-Natta catalyst for alkene polym. The Cp₂TiCl₂/Sm system reduces sulfoxides to sulfides, benzyl halides to bibenzyls and α -bromoketones to ketones. Catalyses pinacol coupling of aldehydes by Mn powder with diastereoselectivity

Biological Use/Importance: Used in DNA-metal binding; possesses antitumour activity

Physical Description: Bright red acicular cryst. (toluene)

Melting Point: Mp 289°

Solubility: Sol. toluene, CHCl₃, EtOH; spar. sol. H₂O, petrol, C₆H₆, Et₂O, CS₂, CCl₄

Aldrich: 23482-6

Fluka: 89530

Rare Chemicals Library: S43940-1

References: