



>>Entry Name: Titanium chloride (TiCl₄)

Synonym(s): Titanium tetrachloride

CAS Registry Number: 7550-45-0

TiCl₄

Molecular Formula: Cl₄Ti

Molecular Weight: 189.691

Accurate Mass: 187.823355

Percentage Composition: Cl 74.76%; Ti 25.24%

Source/Synthesis: Commercially available. Manuf. by passing Cl₂ over TiO₂ and C at 550°. CCl₄ will chlorinate TiO₂

Use/Importance: There is a vast literature dealing with TiCl₄ in alkene polym. catalysts, e.g. in combination with AlCl₃. Lewis acid catalyst; powerful dehydrating agent; in combination with DBU, effects conversion of epoxides to chlorohydrins; with 2,2,6,6-tetramethylpiperidine effects intramolecular cyclisation of (Z)-allylic alcohols; with Zn, generates low-valent Ti spp. for carbonyl coupling and redn. of sulfoxides; used with CH₂Br₂/Zn to generate Lombardo's reagent or with CH₂I₂/Zn for methylenation of ketones and aldehydes; with LiAlH₄, used for generation of dihalocarbenes, deoxygenations

Physical Description: Colourless, readily hydrol. liq.

Melting Point: Mp -24°

Boiling Point: Bp 136°

Solubility: Sol. THF, toluene, CH₂Cl₂

Hazard & Toxicity: HCl is formed on hydrol., incl. in air. Irritant

Aldrich: 34569-5

Fluka: 89542

>>Derivative: Dimer

Synonym(s): Di-μ-chlorohexachlorodititanium(IV), 11Cl

CAS Registry Number: 21790-55-6

Molecular Formula: Cl₈Ti₂

Molecular Weight: 379.382

Accurate Mass: 375.64671

Percentage Composition: Cl 74.76%; Ti 25.24%

Source/Synthesis: Present in liq. TiCl₄ and in TiCl₄ trapped in an argon matrix

Other Data: Dimer, with two chlorine bridges; the exact geometry (tbp or other) is uncertain. This sp. may exist in TiCl₄ at r.t. and Ar matrices at low temps.

References:

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1688B, (ir)

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Rytter, E. *et al.*, *Inorg. Chem.*, 1985, **24**, 639, (Raman, matrix isol, dimer)

Subramanian, V. *et al.*, *Inorg. Chem.*, 1993, **33**, 357, (electronic struct, MS-X_α)

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