>>**Entry Name: Titanium chloride ($TiCl_3$),** 11Cl
Synonym(s): Titanium trichloride

CAS Registry Number: 7705-07-9

$TiCl_3$

Molecular Formula: Cl_3Ti
Molecular Weight: 154.238
Accurate Mass: 152.854503
Percentage Composition: Cl 68.96%; Ti 31.04%

of face-sharing octahedra. Milling the α-form causes rotation of Cl-Ti-Cl sheets through up to 60° and enhances catalytic activity
Source/Synthesis: The α-form results from H_2 reduction of $TiCl_4$ vapour above 500°. The β-form is synth. from $TiCl_4$ and R_3Al. Manuf. from ilmenite. Available commercially
Use/Importance: A very substantial interest is in alkene polym. catalysts. Powerful reducing agent, e.g . $NO_3^{(-)} \rightarrow NH_3$. Used, for example, with $LiAlH_4$, K, Zn/Cu couple, to generate low-valent Ti spp. which effect reductive coupling of carbonyls to vicinal diols and alkenes
Physical Description: α-form is a red-violet solid, β-form is a brown solid. The $\beta \rightarrow \alpha$ transformation occurs at 250-300° or at 40-80° in an inert solv. containing $TiCl_4$. Disproportionates to $TiCl_2$ and $TiCl_4$ above 475°. Readily oxidised in air
Melting Point: Mp 440 dec.°
Solubility: Sol. H_2O, alcohols; insol. Et_2O, $CHCl_3$, CCl_4, CS_2, C_6H_6
Other Data: Paramagnetic, $\mu_{eff} = 1.31\mu_B$ (300K), Néel temp. 165K
Hazard & Toxicity: Flammable, corrosive

Aldrich: 22097-3
Fluka: 89488
Sigma: T3279

>>**Derivative:** Trihydrate

Molecular Formula: $Cl_3H_6O_3Ti$
Molecular Weight: 208.284
Accurate Mass: 206.886198
Percentage Composition: Cl 51.06%; H 2.90%; O 23.04%; Ti 22.99%
Source/Synthesis: Synth. from wet Ph_4PCl + $TiCl_3$ in Me_2CO
Physical Description: Green cryst. + Ph_4PCl + 2 Me_2CO
Other Data: Octahedral Ti, three aqua ligands at *fac* positions

>>**Derivative:** Sesqui-DME complex

Molecular Formula: $C_6H_{15}Cl_3O_3Ti$
Molecular Weight: 289.421
Accurate Mass: 287.956623
Percentage Composition: C 24.90%; H 5.22%; Cl 36.75%; O 16.58%; Ti 16.54%
Source/Synthesis: Synth. from $TiCl_3$ and DME
Use/Importance: Used for the deoxygenative McMurry compling of aldehydes and ketones to give alkenes
Physical Description: Air-sensitive fluffy, blue cryst.

References:

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