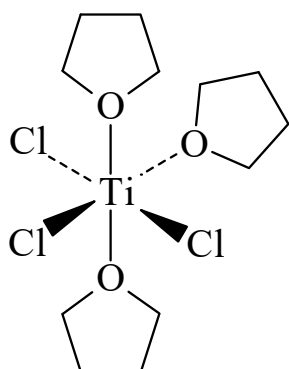




>>Entry Name: Trichlorotris(tetrahydrofuran)titanium(III), 11Cl

Synonym(s): Titanium(III) chloride tris(tetrahydrofuran)



CAS Registry Number: 18039-90-2

Molecular Formula: C₁₂H₂₄Cl₃O₃Ti

Molecular Weight: 370.558

Accurate Mass: 369.027048

Percentage Composition: C 38.90%; H 6.53%; Cl 28.70%; O 12.95%; Ti 12.92%

Source/Synthesis: Synth. by dissolving TiCl₃ in dry THF

Use/Importance: Popular starting material Ti(III) chemistry. Used after reaction with Mg to fix nitrogen via Mg₃N₂ and also as catalyst in polym. of alkenes and reduction of carbonyl compds. to alkenes. Catalyses the McMurry pinacol coupling of aldehydes and ketones giving trimethylsilylated diols

Physical Description: Solid

Aldrich: 46070-2

>>Variant: *mer*-form

CAS Registry Number: 31168-87-3

Molecular Formula: C₁₂H₂₄Cl₃O₃Ti

Molecular Weight: 370.558

Accurate Mass: 369.027048

Percentage Composition: C 38.90%; H 6.53%; Cl 28.70%; O 12.95%; Ti 12.92%

Physical Description: Pale blue air-sensitive solid, dec. by most donor solvs.

Melting Point: Mp 250°

Solubility: Sol. THF, insol. pentane

Other Data: Paramagnetic, $\mu_{\text{eff}} = 1.72\mu_{\text{B}}$ (298K), $1.52\mu_{\text{B}}$ (80K)

References:

Clark, R.J.H. *et al.*, *J.C.S.*, 1963, 379, (*magnetism, uv*)

Jezowska-Trzebiatowska, B. *et al.*, *J. Organomet. Chem.*, 1973, **61**, C43, (*use, CO fixing system*)

Ger. Pat., 1975, 2 515 211; *CA*, **84**, 74876w, (*use*)

Tyrlik, S. *et al.*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1976, **24**, 341, (*use, N₂ fixing system*)

Handlovic, M. *et al.*, *Acta Cryst. B*, 1981, **37**, 811, (*cryst struct, mer-form*)

Inorg. Synth., 1982, **21**, 137, (*synth, ir*)

Hawker, P.N. *et al.*, *J.C.S. Dalton*, 1983, 1123, (*use*)

Synthetic Methods of Organometallic and Inorganic Chemistry, (ed. Hermann, W.A.), Thieme, 1996, **1**, 91, (*synth*)

Lipski, T.A. *et al.*, *J.O.C.*, 1997, **62**, 4566-4567, (*use, pinacol coupling*)