TDC

Titanocene Dichloride, bis(cyclopentadienyl titanium dichloride)

TDC is used as a hydrogenation catalyst for rubber, as a primary catalyst for olefin polymerization reactions, and for organic synthesis reactions.

CAS number
1271-19-8

EINECS/ELINCS No.
215-035-9

TSCA status
listed on inventory

Molecular weight
249.0

Molecular formula
Cp_2TiCl_2

Specifications

Chloride	28.2-28.8%
Purity	≥ 99.5 %
Titanium (IV)	19.0-19.5 %

Characteristics

Appearance	Red crystalline powder
Density, 25 °C	1.60 g/cm^3
Melting point	287-289 °C
Poured bulk density	≈ 0.0005 g/l
Solubility	Soluble in aromatic hydrocarbons, tetrahydrofuran, halogenated solvents and acetonitrile

Notes:
Typical composition: the product has a very high purity and consistency, namely > 99.8% purity based on 1H-NMR. Ti-content 19.0-19.5% wt Cl-content 28.2-28.8% wt 1H-NMR: 6.56 ppm, singlet (in CDCl3 solvent)

Applications

Hydrogenation of rubbers: Titanocene Dichloride and derivatives are used as hydrogenation catalyst for rubbers, like SBS and SEBS, to improve heat stability and resistance to ozone/oxidation [1]. Polymerization: Titanocene Dichloride can be used with polymethylaluminoxane as a catalyst for metallocene type olefin polymerizations [2]. Organic synthesis: Titanocene Dichloride is a useful reagent for a wide variety of synthetic transformations. It can be used with Grignard reagents for the reduction of aryl and vinyl halides [3]; with magnesium for the reduction of organic halides, azo compounds, haloketones, and haloesters [4]; with sodium for the reduction of aliphatic aldehydes, esters, and epoxides [5]; for the reductive decyanation of alkyl nitriles [6]; and the reduction of olefins [7]. Titanocene Dichloride has been used with alkylaluminum compounds for the alkylation of α-olefins [8] and alkynylsilanes [9]. It can be reacted with trimethylaluminum to form Tebbe reagent, which is used to transform a carbonyl into a methylene group [10]. Nouryon can further convert Titanocene Dichloride into derivatives required by the customer, e.g. by substituting the Cl-atoms by other groups or by replacing the cyclopentadienyl rings with substituted cyclopentadienyl rings.

Storage

Store under a nitrogen atmosphere in a cool, dry, well-ventilated area away from flammable materials and sources of heat or flame.

Packaging and transport

TDC is available in industrial volumes and packaged in 170 l cone drums containing 75 kg material or in a plastic bag in a cardboard box with 20 kg material. Custom dedicated packaging can be made available on request. Both packaging and transport meet the international regulations.

Safety and handling

Titanocene Dichloride reacts with water to release hydrogen chloride. Although the reaction is not violent, hydrogen chloride is corrosive and toxic. Protect from atmospheric moisture. Titanocene dichloride is not self-reactive and is stable under most conditions of shipping and handling. Please refer to the Safety Data Sheet (SDS) for further information on the safe storage, use and handling of TDC. This information should be thoroughly reviewed prior to acceptance of this product. The SDS is available at nouryon.com/sds-search

Additional information

See e.g. EP545844B1; EP601953B1; US5583185A; EP885905A1; WO9952918A1; US 5039755. 1) Kaminsky, W.; Miri, M. Proc. Int. Symp. Relat. Homog. Heterog. Catal. 1986, 5, 327-41. 2) Colomer, E.; Corriu, R. J. Organomet. Chem. 1974, 82, 367-73. 3) For example, see: Nelsen, T.R.; Tufariello, J. R. J. Org. Chem. 1975, 40, 3159-60. 4) van Tamelen, E.E.; Gladysz, J.A. J. Am. Chem. Soc. 1974, 96, 5290-1. 5) van Tamelen, E.E.; Rudler, H.; Bjorklund, C. J. Am. Chem. Soc. 1971, 93, 7113-4. 6) van Tamelen, E.E.; Cretney, W.; Klaentschi, N.; Miller, J. S. J. Chem. Soc., Chem. Commun. 1972, 481-2. 7) Barber, J.J.; Willis, C.; Whitesides, G.M. J. Org. Chem., 1979, 44, 3603-4. 8) Eisch, J.J.; Manfre, R.J.; Komar, D.A. J. Organomet. Chem. 1978, 159, C13-9. 9) Tebbe, F. N.; Parshall, G. W.; Reddy, G. S. J. Am. Chem. Soc. 1978, 100, 3611-3.

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