Technical Information

Intermediates

TI/CZ 0001 e February 2008

Page 1 of 4

Supersedes edition dated August 2006



 $@ = {\sf Registered\ trademark\ of\ BASF\ SE}$

Tetrahydrofuran (THF)

CAS Registry No.:

109-99-9



 C_4H_8O

Molar mass 72.1 g/mol

Product Specification

Characteristics	Specification	Method
Assay	min. 99.95 %	GC
Water	max. 100 ppm	DIN 51777-1
Colour	max. 10 APHA	DIN EN 1577

Chemical and Physical Properties

Density	0.887 g/cm ³ (20 °C)	
Appearance	clear, colourless liquid	
Boiling point	66 °C	
Melting point	–108.5 °C	
Flash point	−22 °C (DIN 51794)	
Ignition temperature	230 °C	
Vapor pressure (20 °C)	173 hPa (mbar)	
Critical temperature	267 °C	
Critical pressure	51.2 bar	
Critical density	0.32 g/cm ³	
Critical volume	3.11 cm ³ /g	
Solubility	miscible with H ₂ O	
Electric conductivity	0.5 x 10 ⁻⁸ mho/m	
Dielectic constant	7.6 (20 °C)	

Tetrahydrofuran (THF) is an organic solvent and belongs to the class of (cyclic) ethers. It is a colourless, water-miscible liquid with an ether-like odour. THF is used as a solvent of intermediate polarity for organic substances and as a reaction medium or starting material for various syntheses.

The Reppe process is still the preferred synthetic route to THF; it involves a reaction between acetylene and formaldehyde to 2-butyne-1.4-diol, with subsequent hydrogenation to 1.4-butanediol. Other production processes are based on butadiene, propylene oxide and n-butane. THF can also easily be recovered from off-gas streams and contaminated solvents.

BASF Intermediates has implemented and maintains a Quality Management System according to DIN EN ISO 9001: 2000

Health & Environmental Hazards

THF is considered virtually non-toxic based on animal studies. Overexposure by inhalation, ingestion or skin contact may produce nausea, dizziness, headaches, irritation to eyes, skin, and the respiratory system. THF does not contain residual solvent impurities or heavy metals (Pb, Hg, Cd, Cr⁺⁶). For detailed information on THF exposure limits and health effects, please refer to the Material Safety Data Sheet (MSDS).

Transport, Storage & Handling

Peroxide Formation

Small amounts of peroxide may form in THF following prolonged contact with oxygen or air. Above a peroxide concentration of 0.1 %, THF is subject to explosive decomposition on distillation. To inhibit peroxide building, THF is stabilized with 2.6-di-tert-butyl-p-crescol (BHT).

The concentration of BHT in BASF stabilized THF is 200–350 ppm. In the absence of a stabilizer THF must be stored in an inert gas atmosphere and peroxide content must be determined prior to distillation. If peroxide concentration is higher than 0.05%, the peroxide must be destroyed (e.g. with alkali).

Storage & Handling Precautions

THFis highly flammable. All handling facilities should be designed to minimize the probability of fire; adequate ventilation and air change should be maintained in the working area. Spark-proof motors and tools are required; equipment, transportation vehicles and hose connections must be grounded separately to "drain off" static electricity.

THF storage tanks should be equipped with level indicators. Inspection of all working parts should be made at regular intervals to detect any stoppage or plugging by corrosion or freezing. For cleaning or maintenance work, all traces of the solvent must be removed from the storage system, including the pumps, piping and associated equipment. Rinse water has to be handled properly: THF in water is flammable down to a concentration of 0.3 %.

THF drums can be stored outside plant buildings in a cool place. Once a drum has been opened and some portion of the content removed, the shelf-life becomes limited, even if the nitrogen blanket is restored. For this reason, the remaining content of the drum should be used as quickly as possible.

Material Handling/Sampling

THFcan be handled in ordinary steel drum equipment. However, discolouration can occur from rust. Unalloyed steels, austenitic chromium-nickel steels and aluminium are resistant to corrosion. Tinplate should not be used, because the tin is attacked by THF. For transportation through piping, special attention should be directed toward the seals in pumps and valves. Seamless pipe with gasketed flanges is preferable; for underground piping welded pipes should be used for corrosion protection. All screwed connections should be sealed with a PTFE thread sealant. Flanged, 150 psi (PN20) rating, carbon steel ball valves or butterfly valves are strongly preferred, brass or bronze valves avoided. A wedge ring of PTFE is preferred for valve stem packing.

Special attention should also be directed to sample extraction receptacles. For this purpose, glass bottles with glass plugs or polyethylene bottles with polyethylene screw lids are preferable. As THF permeates through polyethylene, this material should not be used for long-term storage of samples; glass bottles should be used instead. Other materials, such as cardboard insulations in PE lids can be attacked by THF during sample extraction, leading to changes in visual appearance.

Packaging

THF from BASF is available stabilized and non-stabilized in bulk containers and 180 kg steel drums.

Applications

Polytetrahydrofuran (PolyTHF®)

The largest proportion of THF produced is used as a monomer in the production of polytetrahydrofuran (PolyTHF), also known as polytetramethylene ether glycol (PTMEG) or polytetramethylene oxide (PTMO). PolyTHF is an important raw material for the production of elastic textile fibres, thermoplastic polyurethanes, molded elastomers and copolyesters and copolyamides. BASF produces PolyTHF in various molecular weights. With its physical and chemical properties, PolyTHF made by BASF is far superior to comparable materials like polyester polyoles.

Reaction Medium

THF is a reaction medium, used primarily in the pharmaceutical industry, e.g. in Grignard syntheses or lithium aluminium hydride reductions. For these purposes, THF is especially qualified because of its broad solvency for polar and non-polar compounds. Thus, it is the only medium in which many Grignard compounds can be obtained. Because of its good solvent power, THF is also a useful reaction medium for the production of organometallic compounds and anionic polymerization reactions.

Adhesives

THF can be used for the production of PVC adhesives for rigid PVC. It is used as a swelling agent for bonding plasticized PVC film and for fabricating PVC pipe systems.

Coatings & Speciality Coating Systems

The abrasion resistance of video, computer or audio tapes can be improved by applying coatings derived from polyurethane or PVC in which the solvent phase is a blend of THF and toluene. The physical and mechanical properties of cellophane can be improved by applying coatings formulated from polyvinylidene chloride in which the solvent phase is a blend of THF and toluene.

THF allows the preparation of highly concentrated solutions of various polymers. Although THF evaporates rapidly, films formed from its solutions have minimal tendency towards blushing during drying. In the production of liquid crystal displays (LCD), THF is a preferable solvent for the preparation of the coating layer.

Miscellaneous Applications

Its broad solvency capabilities make THF useful for numerous chemical reactions. Some other examples for THF applications are:

- Extraction of some drugs, e.g. alkaloids
- Removal of impurities like wax, fat, or other substances from compounds that are insoluble in THF
- · Production of artificial leather
- Production of gas odourants
- Production of printing inks

Note

The data contained in this publication are based on our current knowledge and experience. In view of the many factors that may affect processing and application of our product, these data do not relieve processors from carrying out their own investigations and tests; neither do these data imply any guarantee of certain properties, nor the suitability of the product for a specific purpose. Any descriptions, drawings, photographs, data, proportions, weights etc. given herein may change without prior information and do not constitute the agreed contractual quality of the product. It is the responsibility of the recipient of our products to ensure that any proprietary rights and existing laws and legislation are observed.

February 2008