WEYLCHEM Wesseling

CYANURIC CHLORIDE

Substance data, handling, safety measures

Contents

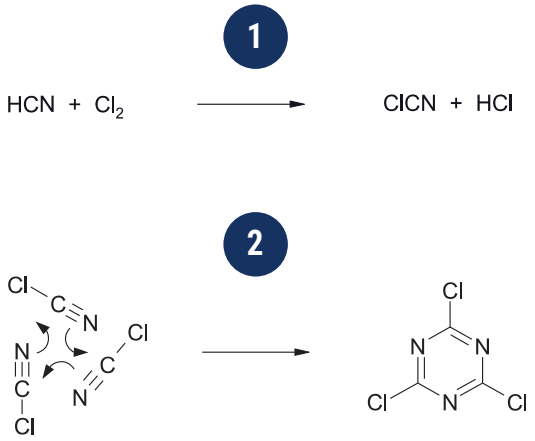
1. Production and grades

1.1 PRODUCTION

Literature sources first mention Cyanuric Chloride in 1827. Its importance as a valuable and versatile intermediate, however, was only recognized in the 1950's. Today, Cyanuric Chloride is one of the most important heterocyclic compounds. The possibility to selectively substitute the three chlorine atoms, coupled with the high stability of the triazine ring, allows for a broad application spectrum (see Chapter 6). WeylChem Wesseling GmbH produces Cyanuric Chloride in Wesseling (Germany).

WeylChem Wesseling GmbH is a leading producer of Cyanuric Chloride worldwide and ensures a high degree of supply security. Cyanuric Chloride is synthesized from cyanogen chloride on a carbon catalyst (Figure 1). Cyanogen chloride itself is derived from a direct synthesis of hydrocyanic acid and chlorine.

Figure 1
Synthesis of Cyanuric Chloride



1.2 PRODUCT GRADES

Cyanuric Chloride is available in different grades and qualities:

- solid N grade (white powder)
- solid N-/F-grade
- liquid L-/N-grade

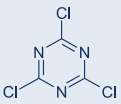
The solid grades are of the same high purity: They only differ in particle size. In order to provide a free flowing material, all solid grades are fluidized with 0.3% of a free flow agent.

For more details please see the Technical Data Sheet or ask for our specification.

Cyanuric Chloride plant in Wesseling (Germany)

2. Substance Data

2.1 IDENTIFICATION OF THE COMPOUND

1.1	Identification numbers	EINECS No.: 203-614-9 CAS No.: 108-77-0 EU-INDEX No.: 613-009-00-5
1.2	EINECS/IUPAC Name	2,4,6-Trichloro-1,3,5-triazine
1.3	Synonyms	Cyanuric Chloride Trichloro-1,3,5-triazine 1,3,5-Triazine-2,4,6-trichloro
1.4	Molecular formula	$C_3Cl_3N_3$
1.5	Structural formula	
1.6	Degree of purity	≥99.5%
1.7	Significant impurities	Hydroxychloro triazines ≤0.5% Cyanuric acid ≤0.5% Free hydrochloric acid ≤0.5%
1.8	Possible additives	free flow additive

2.2 PHYSICO-CHEMICAL CHARACTERISTICS

2.1	Appearance	solid, liquid (hot melt)
2.2	Molecular weight	184.41 g/mol
2.3	Melting point	145 – 146 °C [1, 2]
2.4	Boiling point	193 °C (1013 hPa) [1]
2.5	Density (solid product)	1.92 g/cm³ (20 °C) [3]
2.6	Vapor pressure	ca. 0.025hPa (20 °C)
2.7	Water solubility	44 mg/100 ml (20 °C)
2.8	Flammability	not flammable
2.9	Explosivity	not explosive
2.10	Dangerous reactions	exothermic reaction with water (hydrolysis to form cyanuric acid and hydrogen chloride), dimethyl formamide, alcohols, amines, mercaptans

2.3 CHEMICAL PROPERTIES

2.3.1 SOLUBILITY

Solubility of Cyanuric Chloride in H_2O[4]							
T	[°C]	0	5	10	15	20	25
solubility	[mg/100 ml]	32	35	38	41	44	49

Cyanuric Chloride only slightly dissolves in water. Slow hydrolysis to cyanuric acid and HCl takes place.

Solubility of Cyanuric Chloride in organic solvents (g/100 ml at 25 °C)			
Acetone [4]	25.0	**Dioxane**	55.0
Acetonitrile	21.0	**Ethyl acetate**	21.0
Acrylonitrile	19.0	**Methyl ethyl ketone**	27.0
Benzene	19.0	**Nitrobenzene**	18.0
Chlorobenzene	16.0	**Carbon tetrachloride**	7.5
Chloroform	20.0	**Tetrahydrofuran**	43.0
Diethyl ether	14.0		

Solubility in toluene					
T	[°C]	20	30	40	50
solubility	[g/100 ml]	17.2	19.8	25.0	29.7

2.3.2 REACTIVITY

Cyanuric Chloride is a very reactive compound. Its chemical behavior is comparable to acid chlorides. Its three chlorine atoms can be substituted successively as a function of temperature (Fierz-David Rule [5]).

Reactions include those with alcohols, phenols, sulfides, thiols, amines and other nucleophiles allowing selective synthesis of a multitude of derivatives [6].

2.3.3 HYDROLYSIS

With water, Cyanuric Chloride is hydrolyzed to cyanuric acid [5] (see Chapter 4.6, "Disposal"). The hydrolysis takes place in stages (see Figure 2+3), whereby the three chlorine atoms of the molecule are substituted at different rates under formation of HCl.

The hydrolysis is a strongly exothermic reaction that can be dangerous if it is not run under safe, controlled conditions (see Chapter 5.3, "Dangerous Reactions").

Figure 2
Hydrolysis of Cyanuric Chloride

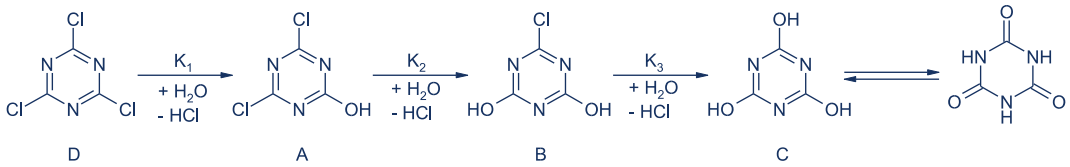
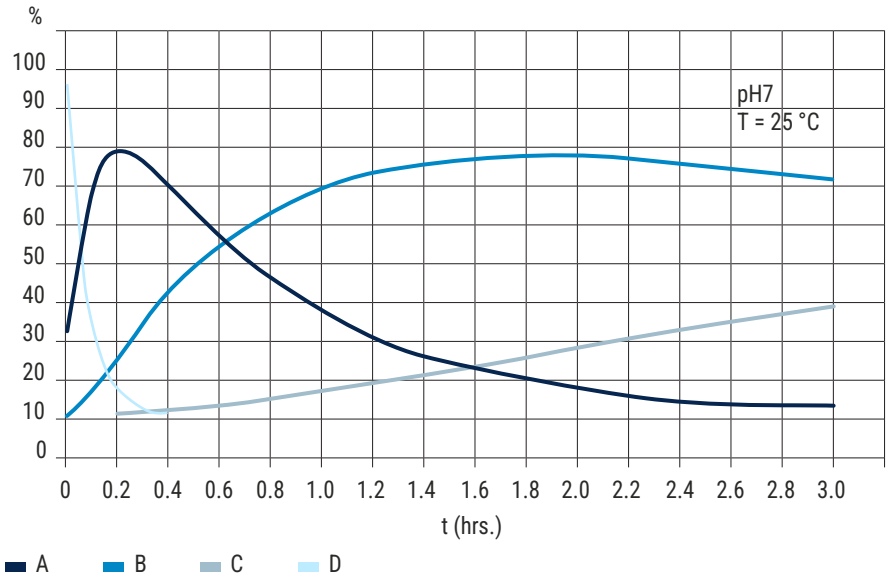


Figure 3
Concentration of the hydrolysis products of Cyanuric Chloride (D) as a function of time at pH 7; at lower pH values the hydrolysis takes place even more rapidly.



3. Handling

3.1 PERSONNEL SAFETY MEASURES

All protective measures given must be strictly adhered to:

- No eating, drinking or smoking during work with Cyanuric Chloride. Before breaks and after finishing work, wash hands and face.
- Respiratory protection: Wear an air purifying respirator during any operation with a potential for release of Cyanuric Chloride. This also refers to the changing of contaminated clothing.
- Hand protection: Wear acid-proof protective rubber gloves.
- Eye protection: Wear basket shaped goggles.
- Body protection: Wear a chemical protective suit.

3.2 HANDLING AND SAFETY

In addition to personal protective clothing the following safety measures have to be observed when handling Cyanuric Chloride:

- Transfer and handle the product in closed systems whenever possible.
- Ensure adequate ventilation or adequate air extraction at the workplace or around working devices.
- Protect the product from moisture and water.
- Avoid the formation of dust and aerosols.
- Take precautionary measures against static discharge.
- Open container carefully as it may be under pressure (HCl formation by traces of moisture in the product).
- Avoid contact with skin, eyes and clothes.
- Change moistened or saturated work clothes.
- Respiratory protection is recommended while handling Cyanuric Chloride.

3.3 FIRST AID

In case of specific contact with Cyanuric Chloride the following instructions must be observed:

- **Following inhalation:** Possible symptoms are: Severe irritation of the mucous membranes (nose, throat, eyes), cough, sneezing, lacrimation. The development of the symptoms may be delayed. Move affected persons into fresh air. If respiratory distress occurs (severe persistent cough): Maintain patient in a half-seated position with the upper body raised. Seek the assistance of a doctor immediately.
- **Following skin contact:** Rinse immediately with soap and plenty of water. If skin irritation persists, seek medical advice immediately.
- **Following eye contact:** Open the eyes and rinse immediately for 10 minutes with plenty of water. Protect eyes. Call ambulance (cite as cause: Caustic burn to the eye). Ensure an immediate further treatment by an ophthalmologist.
- **Following ingestion:** Do not induce vomiting. Only if injured person is fully conscious, rinse mouth with water. Immediately drink large amounts of water in small sips to induce dilution. Call for medical advice immediately. Information for physicians: Therapy as for chemical burns. After massive inhalation there may be acute bronchitis with obstructive impairment of lung function.

3.4 LABELING

Following European GHS classification Cyanuric Chloride is labeled as follows:

Hazard symbol: GHS 05

Hazard symbol: GHS 06

It is assigned to the following H- and P-phrases:

HAZARD STATEMENT	
H330	Fatal if inhaled.
H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H335	May cause respiratory irritation.

ADDITIONAL SAFETY STATEMENT	
EUH014	Reacts violently with water.

For more details ask for our MSDS or our team of experts.

PRECAUTIONARY STATEMENT: PREVENTION	
P260	Do not breathe dust/fume/gas/mist/vapors/spray.
P280	Wear protective gloves/protective clothing/eye protection/face protection.
P284	In case of inadequate ventilation wear respiratory protection.

PRECAUTIONARY STATEMENT: REACTION	
P302 + P350 IF ON SKIN:	Wash with plenty of water/soap.
P305 + P351 + P338 IF IN EYES:	Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER or doctor/physician.

PRECAUTIONARY STATEMENT: STORAGE	
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.

4. Transportation, packaging and handling support

4.1 TRANSPORTATION REGULATIONS

The following traffic regulations must be observed for the transport of Cyanuric Chloride:

HAZARD STATEMENT	
Land	ADR/RID/GGVSE: Class 8 ADR/RID-Labels: 8 UN-No.2670 PG.:II Orange warning plate: 80/2670
Sea	IMDG Code/GGVSee: Class 8 UN-No. 2670 PG.: II Ems: F-A, S-B
Air*	ICAO-TI/IATA-DGR: Class 8, UN-No. 2670 PG.: II *(for small samples only)

For more information see our latest safety data sheet.

4.2 PACKAGING

Solid Cyanuric Chloride comes in:
1. FIBCs (one-way bulk bags)
2. ISO-Bulk-Container

Liquid Cyanuric Chloride comes in ISO-Tank Containers as hot melt.

Flexible Intermediate Bulk Containers (FIBC) offer a number of advantages, facilitating transportation, storage and handling:

- Flexible filling weights between 300 and 1000 kg
- Low investment for handling and discharging
- Easy and cost effective handling with fork-lift truck or chain hoist
- Improved work hygiene time and cost
- Savings due to fast discharging and solid waste reduction (95% compared to drums)

ISO Bulk Containers which can be filled with up to 25 metric tons of Cyanuric Chloride offer the advantage of a complete closed system.

Heatable ISO Tank Containers are used for transportation of molten Cyanuric Chloride. This type of packing is available only for transport of liquid Cyanuric Chloride.

For further information on any of the packaging please call our team of experts.

4.3 HANDLING SUPPORT

To facilitate a safe and economic handling of Cyanuric Chloride and to improve working hygiene WeylChem Wesseling has developed a variety of handling solutions and offers technical assistance in meeting individual customer requirements.

4.4 STORAGE

Cyanuric Chloride should always be stored in a dry, cool and well ventilated area. Direct sunlight should be avoided.

The chemical behaviour of Cyanuric Chloride does not change during storage. However, on prolonged storage, pressure and high temperatures can cause agglomeration and lump formation. Storage time should therefore not exceed 6 months.

Under the influence of moisture, Cyanuric Chloride is hydrolyzed, releasing hydrochloric acid. This process is accelerated at higher temperatures. Traces of Cyanuric Chloride in the storage area can cause a very corrosive atmosphere. Spilled Cyanuric Chloride must be removed immediately.

Precautions should be taken to avoid damage to the packaging during handling and storage.

4.5 MATERIALS

Both Cyanuric Chloride solid and liquid can be stored in stainless steel- and aluminum alloy containers and tanks. To protect the outside walls, we recommend the use of a coating of tar-epoxy resin with a thickness of 450 µm. As sealing material, Hostaflon, Gylan, Gore-Tex and graphite have been proven.

Based on possible hydrolysis reactions and concomitant release of hydrogen chloride, high quality materials, e.g. Hastelloy C, titanium, and glass lined are recommended for equipment used for processing Cyanuric Chloride in aqueous solutions.

4.6 DISPOSAL

Disposal of used packaging: Residues of Cyanuric Chloride must be removed (hydrolyzed) before the disposal of the packaging. We recommend a solution of caustic soda which forms water-soluble 2-chloro-4,6-dihydroxy-1,3,5-triazine. Since the hydrolysis of organic chlorine is not complete the AOX-value (absorbable organic halides) has to be considered for disposal of the solution. Complete hydrolysis of Cyanuric Chloride can only be obtained in acidic medium which results in insoluble cyanuric acid. Cyanuric acid has been identified as a natural compound of soil (6a).

SAFETY PRECAUTION*:

Hydrolysis of Cyanuric Chloride is an exothermic reaction. The maximum heat formation of the reaction is 3200 kJ/kg. In order to avoid temperature increase, the ratio of caustic soda solution as well as of hydrochloric acid to Cyanuric Chloride should not be less than 50:1. Used Bulk Bags should be disposed by incineration in accordance with local regulations. If incineration is not possible Bulk Bags must be cleaned under special precautions. Due to the aluminum laminated liner H_2 can be formed by acid or alkaline solution. Under no circumstance should one-way packaging be re-used, either in connection with other applications or to pack or store other substances.

** see also chapter 5.3. dangerous reactions*

To facilitate a safe and economic handling of Cyanuric Chloride and to improve working hygiene, WeylChem Wesseling GmbH has developed a variety of handling solutions and offers technical assistance in meeting individual customer requirements.

5. Emergency measures

5.1 IN CASE OF ACCIDENTAL RELEASE

Personal precautionary measures:
Wear full protective equipment described under section 3.1 including a gas mask with minimum A2 B2-P3-filter and do not inhale dust or aerosols and a protective suit.

Environmental protection measures:
Do not allow substance to leak into soil, waterways, sewage systems or ground water.

Procedures for cleaning/absorption:

- Use mechanical means to absorb or collect spilled Cyanuric Chloride and store it in a suitable container.
- Flush residues with large amounts of water.
- Dispose of contaminated material as waste according to local legislation.

5.2 IN CASE OF FIRE

Cyanuric Chloride is not flammable. In case of fire close to Cyanuric Chloride, suitable extinguishing media are water mist, powder extinguishers and foam. The use of a full-jet water hose is not suitable (dust formation). The formation of traces of toxic substances such as cyanogen chloride cannot be excluded under certain combustion conditions.

Special protective equipment: In the event of fire, a closed respiratory system independent from circulating air and a protective suit must be worn.

Additional precautions: Water used for extinguishing must not be allowed to leak into soil, sewage, drainage systems or waterways. Contaminated water and fire residues used for extinguishing must be disposed of according to local legislation.

Ignition behavior, fire hazard: Pure, solid Cyanuric Chloride cannot be ignited in air. Cyanuric Chloride dust/air mixtures (1.2 kg Cyanuric Chloride/m^3) cannot be made to explode through a high energy, booster detonation (up to 10 kJ).

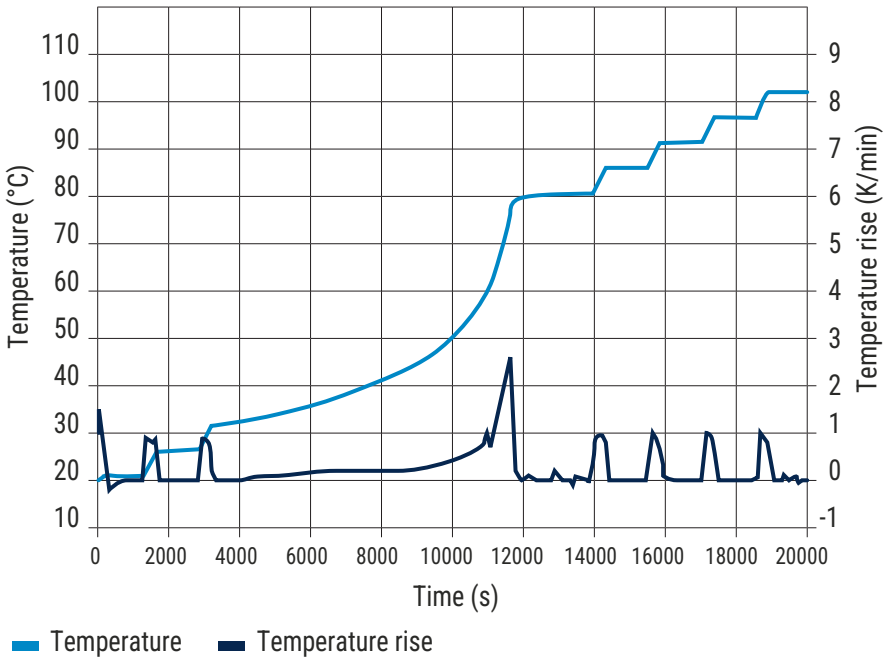
Electrostatic charging of product and packaging is possible. Safety measures against electrostatic discharge have to be taken in hazardous areas. For information on electrostatically dissipative packaging please call our team of experts.

5.3 DANGEROUS REACTIONS

Cyanuric Chloride can react very violently with N,N-dimethyl formamide, dimethyl sulfoxide and allyl alcohol. Also reactions with nucleophiles such as water or other alcohols or even ketones have to be controlled carefully. If, for instance, in case of a reaction with water, temperature and pH values are not regulated or if the Cyanuric Chloride: water ratio is too high, an uncontrollable autocatalytic reaction with formation of HCl can take place (see Figure 4).

If Cyanuric Chloride is hydrolyzed in alkaline solutions or if bases are used for neutralization of HCl during reaction with other nucleophiles the neutralization enthalpy has to be considered and measures for adequate cooling have to be taken. If carbonates are used for neutralization, excess pressure must be expected due to the development of CO_2. Conversions in or with methanol, especially at higher temperatures, can result in a rapid increase in pressure due to the undesirable evolution of methyl chloride.

Figure 4
Hydrolysis of Cyanuric Chloride Temperature increase over time recorded by calorimetry
(heating rate 5 °C/25 min up to 35 °C, above 35 °C adiabatic conditions) (10% CYC in water)



6. Applications

6.1 CROP PROTECTION

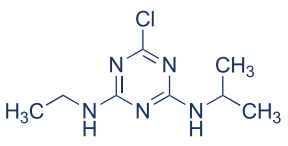
Cyanuric Chloride is key raw material widely used for the synthesis of efficient triazine herbicides. Examples are Terbuthylazine, Atrazine (see Formula 1) and Simazine which are applied for the treatment of broadleaf and grassy weeds in corn, sugarcane, sorghum and pine cultures.

6.2 OPTICAL BRIGHTENERS

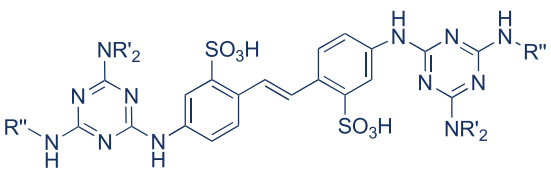
Another important application of Cyanuric Chloride is the synthesis of optical brighteners. These are compounds which absorb invisible UV-light and emit visible light primarily in the blue spectral range. The bluish fluorescence generated lets the yellow or yellowish substrates appear whiter.

Optical brighteners are used in the manufacture of highly refined paper, detergents as well as for the finishing of textiles.

The synthesis of optical brighteners proceeds preferably via the reaction of Cyanuric Chloride with 4,4'-diaminostilbene-2,2'-disulfonic acid and other amines replacing the chlorine substituents of the triazine rings (see Formula 2).



1 Atrazine



2 Core structure of CYC-based optical brightening agents (OBAs)

6.3 REACTIVE DYES

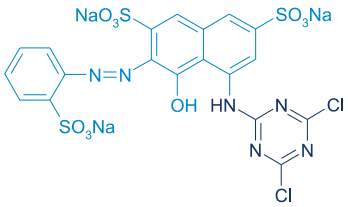
Cyanuric Chloride is an important raw material for the production of numerous dyes. Reactive dyes form a chemical bond with cellulose, the main component of cotton fibers. Other fibers which have nucleophilic groups can also enter into a covalent bond with the triazine substituents, i.e. the dye is chemically fixed on the fiber. The result is a high-grade, non-fading, colorfast dyeing.

6.4 UV LIGHT STABILIZERS

Cyanuric Chloride is a main component in the synthesis of UV light stabilizers, which are used frequently in plastics. The UV light stabilizers are either UV absorbers or radical scavengers like e.g. the hindered amine type (HALS). They improve the functional life time of plastic materials and prevent discoloration and brittleness. The plastics with UV light stabilizers are therefore widely used, among other applications, in the automotive industry. Moreover, UV absorbers are used in personal care products like cosmetics and sunscreen.

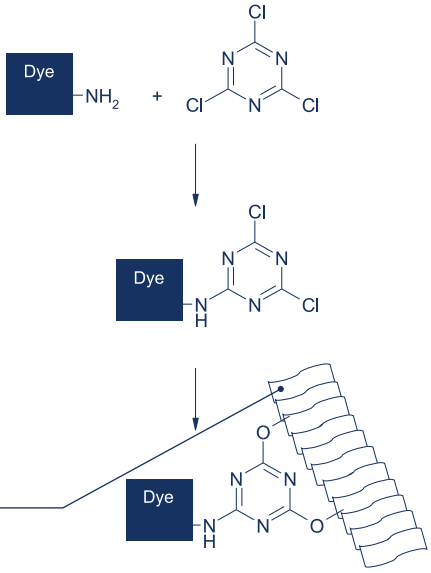
1

Example of reactive dye:
light blue part = chromophor;
deep blue = Cyanuric Chloride anchor.



2

Chemical bonding of a reactive dye
to a cellulose fiber (schematic).



6.5 CROSSLINKERS FOR RUBBER AND PLASTIC

TAC and the TAICROS® product family are a group of WeylChem Wesseling GmbH crosslinkers based on the triazine structure of Cyanuric Chloride. All products are highly efficient trifunctional crosslinking additives for peroxide or electron beam-curing of various materials. In the photovoltaic industry, TAC and TAICROS® help reduce costs by increasing cure speed and improving material properties in high-end electronics applications.

6.6 FURTHER APPLICATIONS

The versatile properties of Cyanuric Chloride are also used in the production of:

- Flame retardants
- Textile auxiliaries
- Lubricants
- Oil additives
- Pharmaceuticals

For a selection of publications on reactions of Cyanuric Chloride and its derivatives please turn to the literature listing seen below.

Literature references relating to specific topics can be provided upon request.

LITERATURE

1) H. Herlinger, Angew. Chem. 76, 437 (1964)
2) C. R.Witschonke, Anal. Chem. 26, 562 (1954)
3) W. Hoppe, Z. Kristallogr. 108, 321 (1957)
4) Gmelin Handbuch der anorg. Chemie, 8. Aufl.; Kohlenstoff, Teil D3, 272, Springer Verlag (1976)
5) H. Fierz-David, M. Matter; J. Soc. Dyers and Colorists 53, 424 – 36 (1937)
6a) E. Smolin, L. Rapoport: The Chemistry of Heterocyclic Compounds, s-Triazines and Derivatives, Interscience Publishers Inc., N.Y. (1967)
6b) J. Thurston et al., Cyanuric Chloride Deriva tives I-IX, J. Am. Chem. Soc. 73, 2981 (1951)
6c) E. J. Modest in: Heterocyclic Compounds, ed. R.C. Elderfield Wiley, NY (1961), Vol. 7, 666
6d) V. J. Mur, Russ. Chem. Rev. (Engl. Transl.), 83, 31 (1964)
6e) J.M.E. Quirke in: Comprehensive Heterocyclic Chemistry Vol. 3, 460, 482 Pergamon Press, 1. Aufl. (1984)
7) Internal unpublised data
8) D. Mannebeck, M. Schmidt, A. Munder, R. Vormberg, Degussa AG, in: GIT Verlag, 43 (1999) 121 – 124
9) V. M. Blagodatin; Giz. Tr. Prof. Zabol 12, 35 (1968) (russ.)
10a) W. Weigert, G. Dusing, N. Kriebitzsch, H. Pfleger, Degussa AG, in Ullmans Encyclopadie der techn. Chemie, 4. Aufl. Bd. 9, 650, Verlag Chemie, Weinheim (1975)
10b) N. Kriebitzsch, H. Klenk, Degussa AG in Ullmann's Encyclopedia of Industrial Chemistry 5th Edition, Vol A8, (1998), 191 – 200
11) R. A. Jedrychowski; R. Gorny, J. Stetzkiewicz: The Toxicologist, 12 (1992) 119
12) G. Gatenacci; Med. Lav. 78 (1987) 155
13) W. Diller, J. Lewalter, H. P. Hoffarth, H. Merker, B. Rohrich: Symposium der deutschen Gesellschaft fur Arbeitsmedizin e.V., 32. Jahrestagung, Koln (1992) 6
14) E. Alt, W. Diller: Zbl. Arbeitsmed., 38 (1988) 22
15a) P. Morfeld et al.; Zbl Arbeitsmed (2014) 64, 10 – 25; DOI 10.1007/s40664-013-0001-5
15b) P. Morfeld, B. Noll; Zbl Arbeitsmed (2014), 64, 73 – 85 DOI 10.1007/s40664-013-0002-4

WeylChem Wesseling GmbH

Brühler Straße 2 , 50389 Wesseling
Germany
www.weylchem.com

Commercial contact

Mr. Mengbo Ge
mengbo.ge@weylchem.com

Ms. Christina Feußner
christina.feussner@weylchem.com

Technical contact

Ms. Dr. Wibke Hartleb
wibke.hartleb@weylchem.com