

# Safety data for acetonitrile



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[Glossary](#) of terms on this data sheet.

The information on this web page is provided to help you to work safely, but it is intended to be an overview of hazards, not a replacement for a full Material Safety Data Sheet (MSDS). MSDS forms can be downloaded from the web sites of many chemical suppliers.

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## General

Synonyms: cyanomethane, ethyl nitrile, methanecarbonitrile, methyl cyanide, ethanenitrile, USAF EK-488, NCI-C60822, NA 1648.

Molecular formula:  $C_2H_3N$

CAS No: 75-05-8

EC No: 200-835-2

Annex I Index No: 608-001-00-3

## Physical data

Appearance: colourless liquid with ether-like odour

Melting point: -46 C

Boiling point: 80 C

Vapour density: 1.41

Vapour pressure: 72.8 mm Hg at 20 C

Specific gravity: 0.786

Flash point: 6 C

Explosion limits: 4.4% - 16%

Autoignition temperature: 973 F

Critical temperature: 275 C

## Stability

Unstable. Incompatible with alkali metals, acids, bases, reducing agents and oxidizing agents. Highly flammable.

## Toxicology

Harmful if inhaled, swallowed or absorbed through the skin.  
Irritant. Typical STEL 60 ppm. Typical OEL 30 ppm. May cause serious damage to the eyes. Possible teratogen.

### Toxicity data

(The meaning of any abbreviations which appear in this section is given [here](#).)

ORL-RAT LD50 2460 mg kg<sup>-1</sup>

IHL-RBT LC50 2828 ppm/4h.

ORL-RBT LD50 50 mg kg<sup>-1</sup>

SCU-RAT LD50 5000 mg kg<sup>-1</sup>

IVN-RAT LD50 1680 mg kg<sup>-1</sup>

SCU-MUS LD50 4480 mg kg<sup>-1</sup>

ORL-CAT LD50 200 mg kg<sup>-1</sup>

IHL-CAT LC50 18 g m<sup>-3</sup>

### Irritation data

(The meaning of any abbreviations which appear in this section is given [here](#).)

SKN-RBT 500 mg open mld

EYE-RBT 100 microl/24h mod

### Risk phrases

(The meaning of any risk phrases which appear in this section is given [here](#).)

R11 R20 R21 R22 R36.

## Transport information

(The meaning of any UN hazard codes which appear in this section is given [here](#).)

Packing group II. UN No 1648. Hazard class 3.2.

## Personal protection

Safety glasses. Good ventilation.

### **Safety phrases**

(The meaning of any safety phrases which appear in this section is given [here](#).)

S16 S27 S44 S45.

[Return to [Physical & Theoretical Chemistry Lab. Safety home page](#).]

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**Method: ACEN-11**

## Acetonitrile Specification Tests

Last Review: 06/12/07 **HYDROGEN CYANIDE** Page 1 of 5

Next Review: 06/12/11 Reviewed by: Robert Schantz

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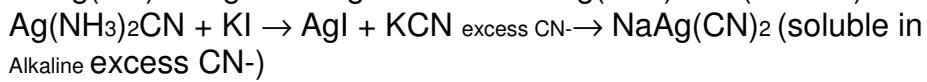
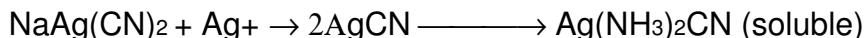
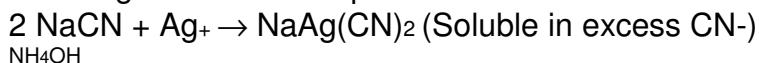
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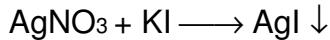
<http://techservice.innovene.com> and select Acetonitrile in "Browse by Product."

### METHOD SUMMARY

Hydrogen cyanide is extracted from the sample as a water soluble salt by means of a solution containing sodium hydroxide, ammonium hydroxide, and potassium iodide. The aqueous extract is then titrated with standard silver nitrate and the following reactions take place:



When all the cyanide ion has been removed from the solution, the first excess drop of the silver nitrate solution will react with the potassium iodide to form an insoluble precipitate.



The hydrogen cyanide content is calculated from the quantity of silver nitrate

required to titrate the sample to the first appearance of silver iodide precipitate.

Repeatability of this method in acetonitrile by the same operator has been measured at the 95% confidence level to be 1.98 ppm. Reproducibility of results between laboratories has not been determined.

### SAFETY

Acetonitrile is hazardous to the health and dangerous to handle. Use acetonitrile in a well ventilated hood. Review the MSDS for detailed information concerning toxicity, first aid procedures and safety precautions. Care should be taken in the

**Method: ACEN-11**

Revision: 5 Final

Revision Date: 12/09/03

## Acetonitrile

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Refer to the appropriate safety section or site manual for the necessary protective equipment to use when handling any reagents or samples.

## **REFERENCES**

STMC-10, "Hydrogen Cyanide in Acrylonitrile and Acetonitrile," SOHIO Test Method, 1976.

ASTM E1178-97 "Standard Test Methods for Analysis of Acrylonitrile"

## **INTERFERENCES**

There are no known interferences to this method.

## **APPARATUS AND REAGENTS**

1. **Separatory funnel**, 250 mL.
2. **Buret**, micro, 10 mL.
3. **Flasks, Erlenmeyer**, 250 mL.
4. **Pipette**, 100 mL, Class A
5. **Flasks, volumetric**, 1000 mL. Class A
6. **Bottle**, plastic, 1000 mL.
7. **Graduated cylinder**, 100 mL, Class A
8. **Balance**, top loading.
9. **Water**, ASTM, Type II.
10. **Silver Nitrate, 0.01N** - The solution may be prepared in the following manner: Dilute 100 mL of 0.1N AgNO<sub>3</sub> [CAS 7761-88-8] (standardized, Fisher SS72 or equivalent) using the 100 mL pipette to one liter with water.
11. **Potassium Iodide**, [CAS 7681-11-0] reagent grade, Fisher P 410 or equivalent.
12. **Sodium Hydroxide**, [CAS 1310-73-2] reagent grade, Fisher S318 or equivalent.

### **Method: ACEN-11**

Revision: 5 Final

Revision Date: 12/09/03

## **Acetonitrile**

### **Specification Tests**

Last Review: 06/12/07 **HYDROGEN CYANIDE** Page 3 of 5

Next Review: 06/12/11 Reviewed by: Robert Schantz

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13. **Ammonium Hydroxide**, [CAS 1336-21-6] ACS reagent, Fisher A669 or equivalent.

14. **Caustic - Iodide Solution** - The solution should be prepared in the following order: Dissolve 3.6g  $\pm$  1g of potassium iodide and 44.1g of sodium hydroxide in 700 mL of water. After these are dissolved and mixed,

add 180 mL of concentrated ammonium hydroxide and dilute to one liter with water and mix. Solutions are stable for at least six months. When larger quantities are needed, it may be prepared in one of the following ways:

- a. To make 45 gallons of solution: Dissolve 612g  $\pm$  1.0g of potassium iodide and 7500g  $\pm$  5g of sodium hydroxide in 31.5  $\pm$  0.5 gallons of water. After these are dissolved and mixed, add 8.1  $\pm$  0.1 gallons of concentrated ammonium hydroxide. Dilute to 45  $\pm$  .5 gallons with water and mix.
- b. To make 40L of solution: Dissolve 144g of potassium iodide and 1764g of sodium hydroxide in 27L of water. After these are dissolved and mixed, add 7200 mL of concentrated ammonium hydroxide. Dilute to 40L with water and mix.

### **CALIBRATION**

The silver nitrate titrant is prepared from a purchased volumetric standard, which is standardized against NIST reference material (See the ACS Reagent Chemicals reference for calibration procedure). Under normal circumstances it is not necessary to re-standardize this titrant.

### **PROCEDURE**

1. Add 100 mL of caustic iodide to a 250 mL Erlenmeyer flask using the graduated cylinder.
2. Blank the caustic iodide by slowly titrating with 0.01N AgNO<sub>3</sub> to a slight opalescence that persists.
3. Transfer the contents of the Erlenmeyer flask to 250 mL separatory funnel. Add 100 mL of sample with a graduated cylinder. CAUTION: Avoid breathing acetonitrile vapors or ammonia vapors from the caustic iodide reagent. Use a well ventilated hood.

#### **Method: ACEN-11**

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4. Stopper and shake the separatory funnel for 1 minute  $\pm$  10 seconds: Be sure to vent the funnel to relieve pressure. Then let the funnel stand in a holder until the layers separate.
5. Draw off the bottom (aqueous) layer into a 250 mL Erlenmeyer flask.
6. Slowly titrate contents of the Erlenmeyer flask with standard 0.01N AgNO<sub>3</sub> until an opalescence is obtained. Record this volume of AgNO<sub>3</sub>.

### **CALCULATIONS**

Calculate the ppm HCN in the sample as follows:

$$\text{HCN, ppm} = \frac{(\text{mL AgNO}_3) (\text{N AgNO}_3) (0.054) \times 10^6}{(\text{mL sample}) (0.78)}$$

Where: 0.054 = milliequivalent wt of HCN

0.78 = specific gravity of acetonitrile

### **REPORT**

Report ppm HCN to the nearest 0.1 ppm.

Example: HCN, ppm = 4.1