

**Summary of Initial Risk Assessment Report**

**Acetonitrile CAS No : 75-05-8**

PRTR No of Japan: 12

This substance is assessed based on Guideline for Initial Risk Assessment Version 1.0

## **1. General Information**

### **1.1 Physico-chemical properties**

|  |  |
|--|--|
| Appearance                                     | Colorless liquid   |
| Melting point                                  | -45 (degC)   |
| Boiling point                                  | 81.6 (degC)  |
| Water solubility                               | Miscible   |
| Henry's constant                               | 3.49 Pa*m <sup>3</sup> /mol (3.45*10 <sup>-5</sup> atm*m <sup>3</sup> /mol) (25degC, measured) |
| Octanol/water partition coefficient ( log Kow) | -0.34 (measured), -0.15 (estimated)  |
| Soil adsorption coefficient                    | Koc = 5 (estimated)  |

### **1.2 Environmental fate**

|                 |   |
|-----------------|---|
| Bioaccumulation | Low bioaccumulative<br>Bioconcentration factor (BCF): 3.2 (calculated using logKow of -0.34)              |
| Biodegradation  | Readily biodegradable<br>Considered to be biodegradable substance under aerobic and anaerobic conditions. |

|                              |   |
|------------------------------|---|
| Stability in the environment | <p>(In air)</p> <p>Reaction with OH radical:</p> <p>Reaction rate constant is <math>2.63 \times 10^{-14} \text{ cm}^3/\text{molecule-sec}</math>. (25 degC, measured)</p> <p>The half - life is 0.8 - 2 years, given OH radical concentration of <math>5 \times 10^5 - 1 \times 10^6 \text{ molecule/cm}^3</math>.</p> <p>Reaction with ozone:</p> <p>Reaction rate constant is <math>1.50 \times 10^{-19} \text{ cm}^3/\text{molecule-sec}</math>. (25 degC, measured value)</p> <p>The half - life is 2 months, given ozone concentration of <math>7 \times 10^{11} \text{ molecule/cm}^3</math>.</p> <p>Reaction with nitrate radical:</p> <p>Reaction rate constant is less than <math>5.00 \times 10^{-11} \text{ cm}^3/\text{molecule/sec}</math>. (25 degC, measured)</p> <p>Since the half - life when the concentration of nitrate radical is estimated <math>2.4 \times 10^8 \text{ molecule/cm}^3</math> (10 ppt) is calculated for 20 years or more, the reaction with nitrate radical in the troposphere atmosphere can be disregarded.</p> <p>Acetonitrile is not degraded directly by light because photoabsorption is limited to the far-ultraviolet region of the electromagnetic spectrum.</p> <p>(In water)</p> <p>The hydrolysis in aquatic environments can be disregarded, since the hydrolysis half-life is 150,000 years or more at pH 7.</p> |
| Environmental fate           | If released into water, acetonitrile is expected to be removed mainly by volatilization and biodegradation.   |

## 2. Sources of release to the environment

### 2.1 Annual production, import, export and domestic supply in 2002 (ton/year)

| Production | Import      | Export      | Domestic supply | Remarks |
|------------|-------------|-------------|-----------------|---------|
| 7,000      | 500 - 1,000 | 500 - 1,000 | 7,000           | --      |

### 2.2 Uses

Raw material for agricultural chemicals, medical products, fragrances and dyes; extraction agent for antibiotics; solvent for HPLC, etc.; solvent for color film processing; reactive solvent, refinement solvent, organic electrobath for lithium batteries, etc.

### 2.3 Release from the industries within the scope of PRTR system (in 2001)

| Release sources                                       |                              | Air (ton) | Waters (ton) | Soil (ton) | Remarks                      |
|---|------------------------------|-----------|--------------|------------|------------------------------|
| Listed industries                                     | Reported release             | 267       | 8            | 0          | Release to rivers: 6.89 tons |
|   | Release outside notification | 15        | <0.5         | 0          |                              |
| Release outside notification from non listed industry |                              | 16        | 0            | 0          |                              |
| Households  |                              | --        | --           | --         |                              |
| Mobile sources  |                              | --        | --           | --         |                              |
| Total   |                              | 298       | 8            | 0          |                              |

## 2.4 Releases from other sources

It has been reported that acetonitrile is generated by incineration of wood, straw, and other plants.

## 2.5 Main release route

Acetonitrile is expected to be released into the environment mainly during use of the substance or products containing it.

## 3. Exposure Assessment

### 3.1 Measured environmental concentration

| Media                                      | No. of points detected /<br>No. of points measured | No. of samples detected /<br>No. of samples measured | Detection range | 95th percentile | Detection limit | Year of investigation,<br>Institution |
|--|--|--|-----------------|-----------------|-----------------|---------------------------------------|
| Air (microg/m <sup>3</sup> )               | 7/7  | 17/17  | 0.093-1.2       | 1.1             | 0.0008-0.076    | 2001<br>Ministry of the Environment   |
| River water (microg/L)                     | 0/44   | --   | nd              | --              | 3               | 2000<br>Ministry of the Environment   |
| Sea water                                  | 0/11   | --   | nd              | --              | 3               | 2000<br>Ministry of the Environment   |
| Drinking water (microg/L)(as ground water) | 0/15   | --   | nd              | --              | 3               | 2000<br>Ministry of the Environment   |
| Food                                       | --   | --   | --              | --              | --              | --                                    |

nd: Not detected

For calculation of the 95th percentile, data less than the detection limit are replaced with a value equal to 1/2 of the detection limit.

### 3.2 Estimated environmental concentration

| Media                        | Estimated concentration | Description  |
|------------------------------|-------------------------|--|
| Air (microg/m <sup>3</sup> ) | 0.554                   | Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) ver. 1.0 |
| River water (microg/L)       | 14                      | Calculated by mathematical model / Initial Assessment System for the PRTR chemicals (IAS)                              |

### 3.3 Estimated environmental concentration in water (EEC)

|               |   |
|---------------|---|
| EEC(microg/L) | 1.5   |
|               | The value (1.5microg/L) equal to 1/2 of detection limit was used for the risk assessment, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment in 2000 <sup>1)</sup> . |

### 3.4 Estimated human intake

| Intake route |                | Concentration used for estimation of intake  | Estimated intake (microg/person/day) | Estimated intake (microg/kg-Bodyweight (BW)/day) |
|--------------|----------------|--|--------------------------------------|--|
| Inhalation   | Air            | 1.1 (microg/m <sup>3</sup> )   | 22                                   | 0.44   |
|              |                | The 95 <sup>th</sup> percentile (1.12 microg/m <sup>3</sup> ) of measured concentrations surveyed by the Ministry of the Environment was used for the risk assessment.   |                                      |  |
| Oral         | Drinking water | 1.5 (microg/L)   | 3                                    | 0.06   |
|              |                | Measured concentrations in ground water were used, since measured concentrations in drinking water were not available. The value equal to 1/2 of detection limit was used for the risk assessment, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment.                  |                                      |  |
| Oral         | Food           | 0.00474 (microg/g)   | 0.57                                 | 0.011  |
|              |                | -The concentration in fish was estimated as a product of concentration in sea water and BCF (3.16L/kg).<br>-The value (1.5microg/L) equal to 1/2 of detection limit was used for concentration in seawater, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment in 2000. |                                      |  |
|              | Subtotal       | --   | 3.57                                 | 0.071  |
|              | Total route    | --   | 26                                   | 0.51   |

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version1.0. If adequate measured concentrations are available, they are given priority and used as values for risk assessment. If they are not available, an estimated value calculated using a mathematical model is used.

#### 4. Hazard assessment

##### 4.1 Effects on organisms in the environment

|           | Acute or Chronic | Species   | Endpoint                            | Concentration        |
|-----------|------------------|---|-------------------------------------|----------------------|
| Algae     | Acute            | <i>Lemna minor</i>  | 96 hours NOEC,<br>Growth inhibition | 1,000(mg/L)          |
| Crustacea | Chronic          | <i>Daphnia magna</i>  | 21days NOEC<br>Mortality of parents | 300(mg/L)            |
| Fish      | Chronic          | <i>Oryzias latipes</i>  | 21days NOEC<br>Mortality, Growth    | 102 or higher (mg/L) |
| Key study |                  | Data of crustacea ( <i>Daphnia magna</i> ) was chosen for the key study because effects were observed at the lowest concentration in the hazard assessment. |                                     |                      |

##### 4.2 Human health toxicity

| Toxicity               | Exposure route   | Species | Duration / Dose method | Toxic effects<br>(Key study is underlined)  | NOAEL or LOAEL<br>(converted)  |
|------------------------|--|---------|------------------------|---|--|
| Repeated dose toxicity | Inhalation   | Mouse   | 13 weeks               | <u>Focal or multifocal discoloration, dark brown or black lesions of forestomach, epithelial hyperplasia of forestomach associated with focal ulcers in females,</u><br>hypoactivity, hunched and rigid posture, hepatocellular cytoplasmic vacuolation, increased absolute and relative liver weights, focal or multifocal squamous epithelial hyperplasia and focal ulcers of forestomach | NOAEL100ppm (168 mg/m <sup>3</sup> )<br>(equivalent to 50 mg/kg/day) |
|                        | Oral   | --      | --                     | --  | --   |
|                        | Dermal   | --      | --                     | --  | --   |
|                        | --   | --      | --                     | --  | --   |
| Carcinogenicity        | Evaluation by IARC : This substance has not been evaluated by IARC |         |                        |   |  |
| Genotoxicity           | Unable to determine genotoxicity                                   |         |                        |   |  |

## 5. Risk Assessment

### 5.1 Environmental organisms

| Risk characterization   | EEC<br>(microg/L)  | NOEC *<br>(mg/L) | MOE<br>(NOEC * /EEC) | Product of uncertainty factors | Conclusion           |  |  |  |  |  |
|---|--|------------------|----------------------|--------------------------------|----------------------|--|--|--|--|--|
|   | 1.5  | NOEC: 300        | 200,000              | 50                             | No immediate concern |  |  |  |  |  |
|   | Product of uncertainty factors (UF):<br>Extrapolation from laboratory test (10) * Toxicity data on two nutritional stages (5) = 50 |                  |                      |                                |                      |  |  |  |  |  |
| Recommendation :  |  |                  |                      |                                |                      |  |  |  |  |  |
| The substance is considered to be of no immediate concern for the moment, and low priority of further work. |  |                  |                      |                                |                      |  |  |  |  |  |

NOEC\* means NOEC, LOEC, EC<sub>50</sub>, etc.

### 5.2 Human health

#### 5.2.1 Repeated dose toxicity

| Exposure route   | Intake<br>(microg/kgBW/day) | NOAEL<br>(mg/kgBW/day) | Risk characterization |                                |                       |
|--|-----------------------------|------------------------|-----------------------|--------------------------------|-----------------------|
|  |                             |                        | MOE                   | Product of uncertainty factors | Conclusion            |
| Inhalation   | 0.44                        | 50                     | 110,000               | 500                            | No immediate concern  |
| Oral   | 0.071                       | No adequate data       | Not calculated        | Not calculated                 | Could not be assessed |
| Total  | 0.51                        | 50<br>(Inhalation)     | 98,000                | 500                            | No immediate concern  |
| Product of uncertainty factors (UF): Inhalation/Oral: Interspecies (10) * Intraspecies (10) * Duration of test (5) = 500 |                             |                        |                       |                                |                       |

#### 5.2.2 Reproductive and developmental toxicity

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#### 5.2.3 Carcinogenicity

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#### 5.2.4. Recommendation for Human Health

In terms of inhalation exposure, the substance is considered to be of no immediate concern for the moment, and a low priority of further work. As for oral exposure, a risk assessment was not conducted because of no toxicity data.

## 6. Supplement

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