DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE

CAS N°: 840-65-3
SIDS Initial Assessment Report
for
9th SIAM
(France, June 29-July 1, 1999)

Chemical Name: Dimethyl 2,6-naphthalenedicarboxylate
CAS No: 840-65-3
Sponsor Country: Japan

National SIDS Contact Point in Sponsor Country:
Mr. Kazuhide Ishikawa
Ministry of Foreign Affairs, Japan

HISTORY:
SIDS Testing Plan were reviewed in SIDS Review Process, where the following SIDS Testing Plan was agreed:
no testing ( )
testing ( X ) Water solubility, Vapour pressure, Octanol/water partition coefficient
Stability in water, Biodegradation
Chronic toxicity to daphnia
Acute toxicity, Combined repeat dose and reproductive toxicity
Gene mutation, Chromosomal aberration test in vitro

Deadline for circulation: March 31, 1999
Date of Circulation: March 30, 1999
(To all National SIDS Contact Points and the OECD Secretariat)
SIDDS INITIAL ASSESSMENT PROFILE

<table>
<thead>
<tr>
<th>CAS NO.</th>
<th>840-65-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHEMICAL NAME</td>
<td>Dimethyl 2,6-naphthalenedicarboxylate</td>
</tr>
<tr>
<td>Structural formula</td>
<td><img src="image" alt="Structural formula" /></td>
</tr>
</tbody>
</table>

RECOMMENDATIONS OF THE SPONSOR COUNTRY

The chemical is currently of low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE RECOMMENDATIONS

Dimethyl 2,6-naphthalenedicarboxylate is stable in water ($T_{1/2} = 263$ days at pH 7 at 25°C). This chemical is not readily biodegradable (OECD 301 C: 7% after 28-day) and moderately bioaccumulative (BCF in Carp = 6.1~63).

No toxicity was observed up to the maximum dispersible concentration with a dispersant (THF/HCO-30). For testings in algae, *Selenastrum capricornutum* (72-h EC$_{50}$, 72-h NOEC), in fish, Medaka (96-h LC$_{50}$, 14-day LC$_{50}$ of *Oryzias latipes*), and in daphnid, *Daphnia magna* (24-h EC$_{50}$ for immobilisation), all results were more than 0.1 mg/l, which is the highest concentration that this chemical can be dispersed. For the daphnid reproduction test, 24-h EC$_{50}$ was 0.02 mg/l, which was also the maximum dispersible concentration using a different dispersant (TMF/HCO-50).

Oral LD$_{50}$ of this chemical for rats is more than 2,000 mg/kg. There are no available data for irritation and sensitisation. In an OECD combined repeat dose and reproductive/developmental toxicity study in rats at 30, 100, 300 and 1000 mg/kg/day, no toxic effects were observed. Therefore, NOAEL was considered to be 1000 mg/kg/day for both repeated dose toxicity and reproductive toxicity. This chemical is not genotoxic, based on negative results in bacterial mutation test and chromosomal aberration test *in vitro*.

The production volume is ca. 250 tonnes/year in 1996 in Japan. All of this produced in Japan is used as monomer unit of polyester, and no consumer use is reported.

A generic fugacity model (Mackey level III) shows that this chemical will distribute mainly into the water phase (87.9%) when it is discharged into water.

IF FURTHER WORK IS RECOMMENDED, SUMMARISE ITS NATURE
### FULL SIDS SUMMARY

<table>
<thead>
<tr>
<th>CAS NO: 840-65-3</th>
<th>SPECIES</th>
<th>PROTOCOL</th>
<th>RESULTS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PHYSICAL-CHEMICAL</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1 Melting Point</td>
<td></td>
<td></td>
<td>192.2 °C</td>
</tr>
<tr>
<td>2.2 Boiling Point</td>
<td></td>
<td></td>
<td>&gt; 300 °C</td>
</tr>
<tr>
<td>2.3 Density</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.4 Vapour Pressure</td>
<td></td>
<td>OECD TG104</td>
<td>3.3 x 10^-4 Pa at 25 °C</td>
</tr>
<tr>
<td>2.5 Partition Coefficient (Log Pow)</td>
<td></td>
<td>OECD TG 107</td>
<td>3.5</td>
</tr>
<tr>
<td>2.6 A. Water Solubility</td>
<td></td>
<td>OECD TG 105</td>
<td>0.15 mg/L at 25 °C</td>
</tr>
<tr>
<td>B. pH</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.12 Oxidation: Reduction Potential</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| **ENVIRONMENTAL FATE AND PATHWAY** | | | |
| 3.1.1 Photodegradation | | | |
| 3.1.2 Stability in Water | OECD TG 111 | T1/2 = Stable in pH 4 at 25 °C |
| | | T1/2 = 65.9 days at pH7 at 25 °C |
| | | T1/2 = 1.04 days at pH9 at 25 °C |
| 3.2 Monitoring Data | | None |
| 3.3 Transport and Distribution | Calculated | Release: 100% to Water |
| | (Fugacity Level III type) | In Air 0.7 % |
| | | In Water 87.9 % |
| | | In Sediment 4.4 % |
| | | In Soil 7.1 % |
| | | (local exposure) 1.1 x 10^-5 mg/L (Japan) |
| 3.5 Biodegradation | OECD 301C | 7 % by HPLC after 28 days |
| 3.7 Bioaccumulation | OECD 305C | BCF: 6.1 - 63 |

<p>| <strong>ECOTOXICOLOGY</strong> | | | |
| 4.1 Acute/Prolonged Toxicity to Fish | Oryzias latipes | OECD TG 203 |
| | | LC50(48hr): &gt; 0.1 mg/l |
| | | LC50(96hr): &gt; 0.1 mg/l |
| | | LC50(14 d): &gt; 0.1 mg/l |
| 4.2 Acute Toxicity to Aquatic Invertebrates | Daphnia magna | OECD TG 202 |
| | | EC50(48hr): &gt; 0.1 mg/l |
| 4.3 Toxicity to Aquatic Plants e.g. Algae | Selenastrum capricornutum | OECD TG 201 |
| | | EC50(72hr): &gt; 0.1 mg/l |
| | | NOEC: &gt; 0.1 mg/l |
| 4.5.2 Chronic Toxicity to Aquatic Invertebrates (Daphnia) | Daphnia magna | OECD TG 202 |
| | | EC50(21d,Repro): &gt; 0.02 mg/l |
| | | NOEC: &gt; 0.02 mg/l |
| 4.6.1 Toxicity to Soil Dwelling Organisms | | None |
| 4.6.2 Toxicity to Terrestrial Plants | | None |
| 4.6.3 Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds) | | None |</p>
<table>
<thead>
<tr>
<th>TOXICOLOGY</th>
<th>Species</th>
<th>Method</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1.1 Acute Oral Toxicity</td>
<td>Rat</td>
<td>OECD TG 401</td>
<td>LD$_{50}$ &gt; 2,000 mg/kg b.w.</td>
</tr>
<tr>
<td>5.1.2 Acute Inhalation Toxicity</td>
<td></td>
<td></td>
<td>No data</td>
</tr>
<tr>
<td>5.1.3 Acute Dermal Toxicity</td>
<td></td>
<td></td>
<td>No data</td>
</tr>
<tr>
<td>5.4 Repeated Dose Toxicity</td>
<td>Rat</td>
<td>OECD Combined</td>
<td>NOAEL = 1,000 mg/kg/day</td>
</tr>
<tr>
<td>5.5 Genetic Toxicity In Vitro</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Bacterial Test (Gene mutation)</td>
<td>S. typhimurium E. coli WP2</td>
<td>Japanese TG and OECD TG 471 &amp; 472</td>
<td>- (With metabolic activation)</td>
</tr>
<tr>
<td>B. Non-Bacterial In Vitro Test</td>
<td>Chinese hamster CHL cells</td>
<td>Japanese TG and OECD TG 473</td>
<td>- (With metabolic activation)</td>
</tr>
<tr>
<td>(Chromosomal aberrations)</td>
<td></td>
<td></td>
<td>- (Without metabolic activation)</td>
</tr>
<tr>
<td>5.6 Genetic Toxicity In Vivo</td>
<td></td>
<td></td>
<td>No data</td>
</tr>
<tr>
<td>5.8 Toxicity to Reproduction</td>
<td>Rat</td>
<td>OECD combined</td>
<td>NOAEL = 1,000 mg/kg/day</td>
</tr>
<tr>
<td>5.9 Developmental Toxicity/</td>
<td></td>
<td></td>
<td>No data</td>
</tr>
<tr>
<td>Teratogenicity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.11 Experience with Human</td>
<td></td>
<td></td>
<td>No data</td>
</tr>
<tr>
<td>Exposure</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[Note] Data beyond SIDS requirements can be added if the items are relevant to the assessment of the chemical, e.g. corrosiveness/irritation, carcinogenicity.
1. **IDENTITY**

- **OECD Name:** Dimethyl 2,6-naphthalenedicarboxylate
- **Synonym:** 2,6-Naphthalenedicarboxylic acid dimethyl ester
- **CAS Number:** 840-65-3
- **Empirical Formula:** C\(_{14}\)H\(_{12}\)O\(_4\)
- **Structural Formula:**
  ![Structural formula diagram]
- **Degree of Purity:** 99.91
- **Major Impurity:** None
- **Essential Additives:** None
- **Physical-chemical properties**
  - **Melting Point:** 192.2 °C
  - **Vapour pressure:** 3.3 x 10\(^{-4}\) Pa at 25 °C
  - **Water solubility:** 0.15 mg/L
  - **Log Pow:** 3.5

2. **GENERAL INFORMATION ON EXPOSURE**

2.1 **Production and import**

The production volume of dimethyl 2,6-naphthalenedicarboxylate in Japan is 1,159 tonnes/year in 1995.

2.2 **Use pattern**

All of dimethyl 2,6-naphthalenedicarboxylate produced in Japan is used as monomer unit of polyester, and no consumer use is reported.

2.3 **Other information**

None

3. **ENVIRONMENT**

3.1 **Environmental Exposure**

3.1.1 **General Discussion**

Dimethyl 2,6-naphthalenedicarboxylate is not biodegradable (OECD 301C: Ca.7 % after 28d) and relatively stable in water under acidic condition. Although direct photodegradation is expected
because dimethyl 2,6-naphthalenedicarboxylate has absorption band in UV and VIS region, the data of half-lifetime is not available.

Dimethyl 2,6-naphthalenedicarboxylate is moderately bioaccumulative (BCF 6.1 – 63, Carp).

The potential environmental distribution of dimethyl 2,6-naphthalenedicarboxylate obtained from a generic Mackay level III fugacity model is shown in Table 1. Parameters used for this model are shown as Annex to this report. The results show that, if dimethyl 2,6-naphthalenedicarboxylate is released into water or soil, it is unlikely to be distributed into other compartment. If dimethyl 2,6-naphthalenedicarboxylate is released into soil, it is likely to be distributed in other compartments.

Table 1
Environmental distribution of dimethyl 2,6-naphthalenedicarboxylate Using a generic level III fugacity model

<table>
<thead>
<tr>
<th>Compartments</th>
<th>Release 100% to air</th>
<th>Release 100% to water</th>
<th>Release 100% to soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>11.6 %</td>
<td>0.7 %</td>
<td>0.0 %</td>
</tr>
<tr>
<td>Water</td>
<td>10.3 %</td>
<td>87.9 %</td>
<td>0.4 %</td>
</tr>
<tr>
<td>Soil</td>
<td>77.2 %</td>
<td>4.4 %</td>
<td>99.6 %</td>
</tr>
<tr>
<td>Sediment</td>
<td>0.8 %</td>
<td>7.1 %</td>
<td>0.0 %</td>
</tr>
</tbody>
</table>

As this chemical is used in closed system as a monomer unit of polyester and is not included in consumer products, its release to the environment may occur only from the production cite.

3.1.2 Predicted Environmental Concentration

As dimethyl 2,6-naphthalenedicarboxylate is produced under the well-controlled closed system, amount of release to air phase is negligibly small. The waste of dimethyl 2,6-naphthalenedicarboxylate from the production system is released to water phase after treated its own wastewater treatment plant. Therefore, Predicted Environmental Concentration (PEC) will be calculated only for the water environment.

a. Regional exposure

According to report from a Japanese manufacturer whose production volume is 250 t/y, 146 kg/year (measured) of dimethyl 2,6-naphthalenedicarboxylate are released with 1.35 x 10^10 L/year of effluent into sea. Local Predicted Environmental Concentration (PEC_{local}) is calculated to be 1.1 x 10^{-5} mg/L as a worst case scenario, employing the following calculation model and dilution factor of 1000(default).

\[
\text{Amount of release (1.46 x 10^8 mg/y)} \\
\times \text{Volume of effluent (1.35 x 10^{10} L/y) x Dilution Factor (1000)}
\]

3.2 Effects on the Environments

3.2.1 Effects on aquatic organisms

Acute and chronic toxicity data of dimethyl 2,6-naphthalenedicarboxylate to aquatic organisms are summarized below (Table 2). Toxicity of this chemical seems low because most toxicity data were
higher than > 0.1 mg/l, the maximum dispersible concentration by a dispersant (a mixture of tetrahydrofuran (THF) and HCO-30 (hydrogenated castor oil), 8 % and 92 % each) with final concentration of 100 mg/l (a limit by OECD test guideline). However, HCO-50 was used in the reproduction test of *D. magna*. Because some side effects of HCO-30 appeared in a preliminary reproduction test as decrease in number of offspring and appearance of unhealthy adults. As a result, the maximum dispersible concentration of test substance decreased to 0.02 mg/l by 30 mg/l of dispersant (1.6 mg/l TMF and 28.4 mg/l HCO-50, each) in the reproduction test of *D. magna*.

Predicted No Effect Concentration (PNEC) of this chemical was determined based on the toxicity data obtained by the Environment Agency of Japan, because other data by different organizations were not available. As the lowest toxicity data, 21-d NOEC of *Daphnia magna* (reproduction), > 0.02 mg/l, was adopted (Table 2). The assessment factor of 100 was used according to the OECD Provisional Guidance for Initial Assessment of Aquatic Effects (EXCH/ MANUAL/ 96-4-5.DOC/May 1996), because chronic toxicity data for fish was absent.

As a lowest data 21-d EC50 (> 0.02 mg/l) of *Daphnia magna* was selected.

Thus, PNEC of this chemical is calculated as below

\[
PNEC = \frac{(> 0.02)}{100} = > 0.0002 \text{ mg/l}
\]

**Table 2**

Acute and chronic toxicity data of dimethyl 2,6-naphthalenedicarboxylate to aquatic organisms at different trophic levels. The data were obtained by the Environmental Agency of Japan based on the OECD Test Guide Lines and GLP.

<table>
<thead>
<tr>
<th>Species</th>
<th>Endpoint</th>
<th>Conc. (mg/l)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Selenastrum capricornutum (algae)</td>
<td>Bms 72 h EC50</td>
<td>&gt; 0.1</td>
<td>a, 1), A</td>
</tr>
<tr>
<td></td>
<td>Bms 72 h NOEC</td>
<td>&gt; 0.1</td>
<td>c, 1), C</td>
</tr>
<tr>
<td>Daphnia magna (Water flea)</td>
<td>Imm 24 h EC50</td>
<td>&gt; 0.1</td>
<td>a, 1), A</td>
</tr>
<tr>
<td></td>
<td>Rep 21 d EC50</td>
<td>&gt; 0.02</td>
<td>c, 1)</td>
</tr>
<tr>
<td></td>
<td>Rep 21 d NOEC</td>
<td>&gt; 0.02</td>
<td>c, 1), C</td>
</tr>
<tr>
<td>Oryzias latipes (fish, Medaka)</td>
<td>Mor 96 h LC50</td>
<td>&gt; 0.1</td>
<td>a, 1)</td>
</tr>
<tr>
<td></td>
<td>Mor 14-d LC50</td>
<td>&gt; 0.1</td>
<td>a, 1), A</td>
</tr>
</tbody>
</table>

Notes: Bms; biomass, Mor; mortality, Rep; reproduction, A), C); the lowest values among the acute or chronic toxicity data of algae, Cladocera (water flea) and fishes to determine PNEC of this chemical.

1) Toxicity data of the tests were conducted by the Environment Agency of Japan based on OECD Test Guidelines and GLP.

### 3.2.2 Terrestrial effects

No data available

### 3.2.3 Other effects

No data available

### 3.3 Initial Assessment for the Environment

Predicted No Effect Concentration (PNEC) of this chemical has been calculated as > 0.0002 mg/l.
PEC from Japanese local exposure scenario is \(1.1 \times 10^{-5} \text{ mg/l} \).

\[
\text{PEC}_{\text{local}} / \text{PNEC} = 1.1 \times 10^{-5} / (> 0.0002) = < 0.055 < 1
\]

Therefore, it is currently considered of low potential risk for environments and low priority for further work.

4. **HUMAN HEALTH**

4.1 **Human Exposure**

4.1.1 **Occupational exposure**

Dimethyl 2,6-naphthalenedicarboxylate is produced in closed systems and used for polyester resin synthesis. The occupational exposures are expected through inhalation and dermal route is assumed negligible because this chemical is solid. As the atmospheric concentration in plant was not measured, the maximum exposure levels are estimated according to working schedules as follows. If a single worker (body weight: 70 kg, respiratory volume: 1.25 m\(^3\)/hr) is assigned to implement this operation without protection, the highest daily intake (EHE) is calculated as 0.04 mg/kg/day as the worst case. Practically, workers always wear protective gloves and respiratory protective equipment (mask) during the operation.

<table>
<thead>
<tr>
<th>Frequency</th>
<th>Duration</th>
<th>Working</th>
<th>Maximum Concentration</th>
<th>Maximum EHE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times/day</td>
<td>hr/day</td>
<td>hr/day</td>
<td>mg/m(^3)</td>
<td>mg/kg/day</td>
</tr>
<tr>
<td>Bag Filling</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>0.04</td>
</tr>
</tbody>
</table>

EHE: Estimated Human Exposure

4.1.2 **Consumer exposure**

As dimethyl 2,6-naphthalenedicarboxylate is used as a raw material for polyethylenenaphthalate resin, liquid crystal, engineering plastic, etc., consumer exposure is not expected in sponsor country.

4.1.3 **Indirect exposure via the environment**

As dimethyl 2,6-naphthalenedicarboxylate is persistent in water and moderately bioaccumulative, the exposure to the general population via the environment would be possible through drinking water processed from surface water and through fish which may accumulate this chemical.

The concentration in drinking water should be estimated to be equal to PEC calculated in Section 3.1, i.e. \(1.1 \times 10^{-5} \text{ mg/l} \). The daily intake through drinking water is calculated as \(3.67 \times 10^{-7} \text{ mg/kg/day} \) (2 l/day, 60 kg b.w.).

Using the maximum bioconcentration factor of 63 obtained by tests, the concentration of this chemical in fish can be calculated as follows:
PEC\textsubscript{fish} = (1.10 \times 10^{-5} \text{ mg/l}) \times 63 = 6.93 \times 10^{-7} \text{ mg/g-wet}

As a daily intake of fish in Japan is estimated to be 90 g for 60 kg body weight person, a daily intake of this chemical will be $1.04 \times 10^{-6} \text{ mg/kg/day}$.

### 4.2 Effects on Human Health

a) Acute toxicity

Any lethality in both sexes of rats by oral administration was not observed at dose of 2,000 mg/kg. Any toxic signs did not appear. [MHW, Japan (1997)]

b) Irritation

There are no available data.

c) Sensitisation

There are no available data.

d) Repeated toxicity

[SIDS data] Oral toxicity of dimethyl 2,6-naphthalenedicarboxylate in rats was studied by an OECD combined repeat dose and reproductive/developmental toxicity screening test. The chemical was administered by gavage at doses of 0, 30, 100, 300 and 1,000 mg/kg/day for 45 days in males and from 14 days before mating to day 3 of lactation in females. No effects of the test substance on males or females were noted. The NOAEL for repeat dose toxicity is considered to be 1,000 mg/kg/day for both sexes. [MHW, Japan (1997)]

e) Reproductive/developmental toxicity

[SIDS data] Oral toxicity of dimethyl 2,6-naphthalenedicarboxylate in rats was studied by an OECD combined repeat dose and reproductive/developmental toxicity screening test. The chemical was administered by gavage at doses of 0, 30, 100, 300 and 1,000 mg/kg/day for 45 days in males and from 14 days before mating to day 3 of lactation in females. No effects of the test substance on copulation, fertility, delivery or lactation were noted. The NOAEL for reproductive performance of males and females, and for pup development is considered to be 1,000 mg/kg/day. [MHW, Japan (1997)]

f) Genetic toxicity

Bacterial test

[SIDS data] Dimethyl 2,6-naphthalenedicarboxylate was not mutagenic in *Salmonella typhimurium* TA100, TA1535, TA98, TA1537 and *Escherichia coli* WP2 uvrA, with or without an exogenous metabolic activation system. [MHW, Japan (1997)]

Non-bacterial test *in vitro*

[SIDS data] Genotoxicity of dimethyl 2,6-naphthalenedicarboxylate was studied by chromosomal aberration test in cultured Chinese hamster lung (CHL/IU) cells. Structural chromosomal aberrations were not induced up to a maximum concentration of 2.4 mg/ml (10 mM) with continuous treatment, or by short-term treatment with and without an exogenous metabolic
activation system. Polyploidy was induced by continuous treatment with 2.4 mg/ml for 48 h. However, it was considered that dimethyl 2,6-naphthalenedicarboxylate did not induce chromosomal aberrations or polyploidy since the frequency was very low. [MHW, Japan (1997)]

4.3 Initial Assessment for Human Health

Oral LD₅₀ of dimethyl 2,6-naphthalenedicarboxylate for rats is more than 2,000 mg/kg. There are no available data for irritation and sensitisation. In a combined repeat dose and reproductive/developmental toxicity study, any toxic effects were not observed. Therefore, NOAEL was considered to be 1000 mg/kg/day for both repeated dose toxicity and reproductive toxicity. This chemical may not be genotoxic, based on negative results in bacterial mutation test and chromosomal aberration test in vitro.

Occupational exposure
Dimethyl 2,6-naphthalenedicarboxylate is produced and used in a closed system at industries and workers wear protective gloves and respiratory protective equipment during bag filling operation. As the route of occupational exposure may be an inhalation in limited workers, there is no available data of the atmosphere concentration. Based on the predicted high concentration and the possibility of exposure period, the daily intake is calculated as 0.04 mg/kg/day as the worst case. Occupational risk is presumably low because the margin of safety is 2.50 x 10⁴.

Consumer exposure
No consumer exposure is expected because this chemical is not used in consumer products.

Indirect exposure via environment
As for indirect exposure via environment, PEC₉₉₉ of 1.10 x 10⁻⁵ mg/l from local exposure scenario was used for the estimation. The daily intakes through drinking water and fish are calculated as 3.67 x 10⁻⁷ mg/kg/day and 1.04 x 10⁻⁶ mg/kg/day, respectively. Since the margin of safety is very large, such as 2.73 x 10⁹ for drinking water and 9.62 x 10⁸ for fish, health risk via environment is presumably low.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Dimethyl 2,6-naphthalenedicarboxylate is not biodegradable (OECD 301C: ca. 7% after 28-d) and has relatively stable in water, and moderately bioaccumulative (BCF 6.1~63, Carp). Toxicity values to the test organisms were higher than the maximum dispersible concentrations, > 0.1 mg/l except for > 0.02 mg/l in the reproduction test of Daphnia magna conducted using a different dispersant. PEC/PNEC ratio (1.1 x 10⁻⁴/(> 0.0002) = < 0.55) is less than 1 based on the local exposure scenario in the Sponsor country and NOEC in reproduction test of D. magna. It is currently considered of low potential risk to environments and low priority for further work.

Dimethyl 2,6-naphthalenedicarboxylate is not toxic in a repeated dose and reproductive toxicity studies, and not genotoxic. There is no information on irritation, sensitization and no consumer exposure. The margin of safety is more than 1 x 10⁴ via an occupational and indirect exposure. Therefore, it is currently considered of low potential human risk and low priority for further work.

5.2 Recommendations
No recommendation

6. REFERENCES

Appendix 1

Method for Prediction of Environmental Concentration of Pollutant in Surface Water

1. Predicted environmental concentration in the local environment (PEC_{local}) with effluent release into river

When decomposition, precipitation and vaporization of pollutant can be ignored, it is used that simplified equation by complete mixing model shown with equation (1) to calculate predicted environmental concentration in the local environment (PEC_{local}) as for release effluent into river.

\[
P_{EC_{local}} \text{ (mg/L)} = \frac{C_{0}Q + C_{s}Q_{s}}{Q + Q_{s}} \quad (1)
\]

Where

- \(C_{0}\): Concentration of pollutant in upper stream of release point (mg/L)
- \(C_{s}\): Concentration of pollutant in effluent (mg/L)
- \(Q\): Flow rate of river (m³/day)
- \(Q_{s}\): Flow rate of effluent released into river (m³/day)

At the equation (1), when \(C_{0}\) can be considered as 0, dilution factor of pollutant in the river (R) can be shown with following equation.

\[
R = \frac{C_{s}}{C_{0}} = \left(\frac{Q + Q_{s}}{Q_{s}}\right) \quad (2)
\]

As the worst case, it is used to employ a flow rate at dry season as flow rate of river (Q). When flow rate at dry season is indistinct, it is estimated using the following equation in Japan.

\[
\text{Flow rate at dry season} = \text{mean flow late} / 2.5 \quad (3)
\]

2. Predicted environmental concentration in the local environment (PEC_{local}) with effluent release into sea

For prediction of concentration of pollutant in the sea water with effluent, it is employed generally Joseph-Sendner symbol 146's equation (4). This equation is one of analytic solution led under the following conditions from diffusion equation.

1. It is adopted large area of sea or lake.
2. The flow rate of effluent and concentration of pollutant in the effluent are constant, and distribution of concentration is able to regard as equilibrium state.
3. Effluent is distributed uniformly to vertical direction, and it spreads in a semicircle or segment to horizontal direction.
4. Diffusion coefficient of pollutant at the sea is in proportion to distance from release point of effluent.
5. There is not any effect of tidal current.
6. Decomposition of pollutant can be ignored.
\[
C(x) = (C_s - C(r)) \left(1 - \exp\left(-\frac{Q_s}{d \cdot p \cdot x} \cdot \frac{1}{r}ight)\right) + C(r)
\]  

(4)

Where
- \(C(x)\): Concentration of pollutant at distance \(x\) (m) from release point
- \(C_s\): Concentration of pollutant in effluent
- \(C(r)\): Concentration of pollutant at distance \(r\) (m) from release point
- \(Q_s\): Flow rate of effluent (m\(^3\)/day)
- \(\theta\): Opening angle of seacoast (rad.)
- \(d\): Thickness of diffusion layer (m)
- \(P\): Diffusion velocity (m/day) (1.0  0.5 cm/sec)

When \(C(x)\) is 0 at \(r = \) and density stratification is ignored for simplification, Joseph-Sendner\'s equation (4) is simplified to equation (5)

\[
C(x) = C_s \left(1 - \exp\left(-\frac{Q_s}{d \cdot p \cdot x}\right)\right)
\]  

(5)

Because of \(Q_s/d \cdot p \cdot x \ll 1\) except vicinity of release point, dilution factor \(R(x)\) in distance \(x\) from release point can be shown with equation (6).

\[
R(x) = \frac{C_s}{C(x)} = \frac{d \cdot p \cdot x}{Q_s}
\]  

(6)

When it is employed following parameters in equation (6) as default, dilution factor \(R\) can be shown with equation (7).

- \(P = 1\) cm/sec (860 m/day)
- \(\theta = 3.14\)
- \(d = 10\) m
- \(x = 1000\) m

\[
R = 2.7 \times 10^7/Q_s
\]  

(7)

\(Q_s\): volume of effluent (m\(^3\)/day)
REVISED OECD HPV FORM 1

SIDS DOSSIER
ON THE HPV PHASE 5 CHEMICAL

Dimethyl 2,6-naphthalenedicarboxylate

CAS No. 840-65-3

Sponsor Country: Japan

DATE: March 15, 1999
CONTENTS

Sids Profile

Sids Summary

1. General Information

1.01 Substance Information
   * A. Cas-Number
   B. Name (Iupac-Name)
   * C. Name (Oecd Name)
† D. Cas Descriptor
   E. Einecs-Number
   F. Molecular Formula
* G. Structural Formula
   H. Substance Group
   I. Substance Remark
   J. Molecular Weight

1.02 Oecd Information
   A. Sponsor Country
   B. Lead Organisation
   C. Name Of Responder (Company)

1.1 General Substance Information
   A. Type Of Substance
   B. Physical State
   C. Purity

1.2 Synonyms

1.3 Impurities

1.4 Additives

1.5 * Quantity

1.6 Labelling And Classification (Use And/Or Transportation)

1.7 * Use Pattern
   A. General Use Pattern
   B. Uses In Consumer Products

1.8 Occupational Exposure Limit Value

1.9 * Sources Of Exposure

1.10 Additional Remarks
   A. Options Of Disposal
   B. Other Remarks.

2. Physical-Chemical Data

2.1 * Melting Point

2.2 * Boiling Point

2.3 † Density (Relative Density)

2.4 * Vapour Pressure

2.5 * Partition Coefficient N-Octanol/Water

2.6 * Water Solubility
   A. Solubility
B. Ph Value, Pka Value

2.7 Flash Point (Liquids)

2.8 Auto Flammability (Solid/Gases)

2.9 Flammability

2.10 Explosive Properties

2.11 Oxidising Properties

2.12 ➤ Oxidation: Reduction Potential

2.13 Additional Remarks
    A. Partition Co-Efficient Between Soil/Sediment And Water (Kd)
    B. Other Remarks

3. Environmental Fate And Pathways

3.1 Stability
    3.1.1 * Photodegradation
    3.1.2 * Stability In Water
    3.1.3 Stability In Soil

3.2 * Monitoring Data (Environment)

3.3 * Transport And Distribution Between Environmental Compartments Including Estimated Environmental Concentrations And Distribution Pathways

3.3.1 Transport

3.3.2 Theoretical Distribution (Fugacity Calculation)

3.4 Mode Of Degradation In Actual Use

3.5 * Biodegradation

3.6 Bod-5, Cod Or Ratio Bod-5/Cod

3.7 Bioaccumulation

3.8 Additional Remarks
    A. Sewage Treatment
    B. Other

4. Ecotoxicity

4.1 * Acute/Prolonged Toxicity To Fish

4.2 Acute Toxicity To Aquatic Invertebrates
    * A. Daphnia
    B. Other Aquatic Organisms

4.3 * Toxicity To Aquatic Plants E.G., Algae

4.4 Toxicity To Bacteria

4.5 Chronic Toxicity To Aquatic Organisms

4.5.1 Chronic Toxicity To Fish

4.5.2 (*) Chronic Toxicity To Aquatic Invertebrates
    (E.G., Daphnia Reproduction)

4.6 Toxicity To Terrestrial Organisms

4.6.1 Toxicity To Soil Dwelling Organisms

4.6.2 Toxicity To Terrestrial Plants

4.6.3 Toxicity To Other Non-Mammalian Terrestrial Species
    (Including Birds)

4.7 Biological Effects Monitoring (Including Biomagnification)

4.8 Biotransformation And Kinetics

4.9 Additional Remarks

UNEP Publications 17
5. **Toxicity**

5.1 * Acute Toxicity
   5.1.1 Acute Oral Toxicity
   5.1.2 Acute Inhalation Toxicity
   5.1.3 Acute Dermal Toxicity
   5.1.4 Acute Toxicity By Other Routes Of Administration

5.2 Corrosiveness/Irritation
   5.2.1 Skin Irritation/Corrosion
   5.2.2 Eye Irritation/Corrosion

5.3 Skin Sensitisation

5.4 * Repeated Dose Toxicity

5.5 * Genetic Toxicity In Vitro
   A. Bacterial Test
   B. Non-Bacterial In Vitro Test

5.6 * Genetic Toxicity In Vivo

5.7 Carcinogenicity

5.8 * Toxicity To Reproduction

5.9 * Developmental Toxicity / Teratogenicity

5.10 Other Relevant Information
   A. Specific Toxicities (Neurotoxicity, Immunotoxicity Etc.)
   B. Toxicodynamics, Toxicokinetics

5.11 * Experience With Human Exposure

6. **References**

**Appendix-1**

Note: *; Data Elements In The Sids
†; Data Elements Specially Required For Inorganic Chemicals
### SIDS Profile

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1.01 A.</strong></td>
<td><strong>CAS No.</strong></td>
<td>840-65-3</td>
</tr>
<tr>
<td><strong>1.01 C.</strong></td>
<td><strong>CHEMICAL NAME</strong> <em>(OECD Name)</em></td>
<td>Dimethyl 2,6-naphthalenedicarboxylate</td>
</tr>
<tr>
<td><strong>1.01 D.</strong></td>
<td><strong>CAS DESCRIPTOR</strong></td>
<td></td>
</tr>
</tbody>
</table>
| **1.01 G.** | **STRUCTURAL FORMULA** | ![Structural Formula](image)

#### OTHER CHEMICAL IDENTITY INFORMATION

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1.5</strong></td>
<td><strong>QUANTITY</strong></td>
<td>1,159 tonnes/year in Japan</td>
</tr>
<tr>
<td><strong>1.7</strong></td>
<td><strong>USE PATTERN</strong></td>
<td>Intermediate in closed system</td>
</tr>
<tr>
<td><strong>1.9</strong></td>
<td><strong>SOURCES AND LEVELS OF EXPOSURE</strong></td>
<td>146 kg/year Release into bay</td>
</tr>
</tbody>
</table>

#### ISSUES FOR DISCUSSION (IDENTIFY, IF ANY)

SIDS testing required:
- Water solubility
- Vapour pressure
- Octanol/water partition coefficient
- Stability in water, Biodegradation
- Acute toxicity
- Combined repeat dose and reproductive toxicity
- Gene mutation, Chromosomal aberration test in vitro
## SIDS SUMMARY

**CAS NO:** 840-65-3

<table>
<thead>
<tr>
<th>Study</th>
<th>Information</th>
<th>OECD Study</th>
<th>GLP</th>
<th>Other Study</th>
<th>Radiation N</th>
<th>Acute Study</th>
<th>SIDS Testing Required</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Physical-Chemical Data</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1 Melting Point</td>
<td>Y</td>
<td>N</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>N</td>
</tr>
<tr>
<td>2.2 Boiling Point</td>
<td>Y</td>
<td>N</td>
<td>N</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>N</td>
</tr>
<tr>
<td>2.3 Density</td>
<td>N</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.4 Vapour Pressure</td>
<td>N</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5 Partition Coefficient</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.6 Water Solubility</td>
<td>N</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>pH and pKa values</td>
<td>N</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.12 Oxidation: Reduction potential</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| Environmental Fate and Pathway | | | | | | | |
| 3.1 Photodegradation | N | | | | | | |
| 3.2 Stability in water | N | | | | | | |
| 3.3 Monitoring data | N | | | | | | |
| 3.4 Transport and Distribution | N | | | | | | |
| 3.5 Biodegradation | N | | | | | | |

| Ecotoxicity | | | | | | | |
| 4.1 Acute toxicity to Fish | N | | | | | | |
| 4.2 Acute toxicity to Daphnia | N | | | | | | |
| 4.3 Toxicity to Algae | N | | | | | | |
| 4.5.2 Chronic toxicity to Daphnia | N | | | | | | |
| 4.6.1 Toxicity to Soil dwelling organisms | N | | | | | | |
| 4.6.2 Toxicity to Terrestrial plants | N | | | | | | |
| 4.6.3 Toxicity to Birds | N | | | | | | |

| Toxicity | | | | | | | |
| 5.1.1 Acute Oral | N | | | | | | |
| 5.1.2 Acute Inhalation | N | | | | | | |
| 5.1.3 Acute Dermal | N | | | | | | |
| 5.4 Repeated Dose | N | | | | | | |
| 5.5 Genetic Toxicity *in vitro* | N | | | | | | |
| . Gene mutation | N | | | | | | |
| . Chromosomal aberration | N | | | | | | |
| 5.6 Genetic Toxicity *in vivo* | N | | | | | | |
| 5.8 Reproduction Toxicity | N | | | | | | |
| 5.9 Development / Teratogenicity | N | | | | | | |
| 5.11 Human experience | N | | | | | | |

| Other Toxicity Studies Received | | | | | | | |
| Other P/C Studies Received | | | | | | | |
| Other Environmental Fate Studies Received | | | | | | | |
| Other Ecotoxicity Studies Received | | | | | | | |

20 UNEP Publications
I. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

*A. CAS number 840-65-3

B. Name (IUPAC name) Dimethyl 2,6-naphthalenedicarboxylate

*C. Name (OECD name) Dimethyl 2,6-naphthalenedicarboxylate

†D. CAS Descriptor

E. EINECS-Number 212-661-4

F. Molecular Formula C_{14}H_{12}O_{4}

*G. Structural Formula

\[\text{COOCH}_3\]
\[\text{COOC}_3\]

H. Substance Group

I. Substance Remark

J. Molecular Weight 244.25

1.02 OECD INFORMATION

A. Sponsor Country: Japan

B. Lead Organisation:

Name of Lead Organisation: Ministry of Health and Welfare (MHW)
Ministry of International Trade and Industry (MITI)
Environmental Agency (EA)
Ministry of Labour (MOL)

Contact person: Mr. Kazuhide Ishikawa
Economic International Bureau
Second International Organization Division
Ministry of Foreign

Address:
Street: 2-2-1 Kasumigaseki, Chiyoda-ku, Tokyo 100 Japan
Tel: 81-3-3581-0018
Fax: 81-3-3503-3136

C. Name of responder
Name: Same as above contact person

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

<table>
<thead>
<tr>
<th>Element</th>
<th>Inorganic</th>
<th>Natural Substance</th>
<th>Organic</th>
<th>Organometallic</th>
<th>Petroleum Product</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>[ X ]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

B. Physical State (at 20°C and 1.013 hPa)

gaseous [ ]; liquid [ ]; solid [ X ]

C. Purity

99.91 %

1.2 SYNONYMS

2,6-Naphthalenedicarboxylic acid dimethyl ester

1.3 IMPURITIES

None

1.4 ADDITIVES

None

*1.5 QUANTITY

Remarks: 1,159 tonnes/year
Reference: MITI, Japan

1.6 LABELLING AND CLASSIFICATION

None

*1.7 USE PATTERN

A. General

<table>
<thead>
<tr>
<th>Type of Use:</th>
<th>Category:</th>
</tr>
</thead>
<tbody>
<tr>
<td>main</td>
<td>Intermediate</td>
</tr>
<tr>
<td>industrial</td>
<td>Intermediate in closed system</td>
</tr>
<tr>
<td>use</td>
<td>Intermediate</td>
</tr>
</tbody>
</table>

Remarks: None
Reference: MITI, Japan

1.8 OCCUPATIONAL EXPOSURE LIMIT
* 1.9 SOURCES OF EXPOSURE

In Japan, this chemical is produced in 1 company.

Source: Media of release: Bay
Quantities per media: 146 kg/year
Remarks:
Reference: MITI, Japan

2. PHYSICAL-CHEMICAL DATA

*2.1 MELTING POINT

Value: 192 °C
Decomposition: Yes [ ] No [X] Ambiguous [ ]
Sublimation: Yes [ ] No [ ] Ambiguous [ ]
Method:
GLP: Yes [ ] No [ X ] ? [ ]
Remarks:
Reference: Company data

*2.2 BOILING POINT

Value: > 300 °C
Pressure: 1,018 Pa
Decomposition: Yes [ ] No [ X ] Ambiguous [ ]
Method:
GLP: Yes [ ] No [ X ] ? [ ]
Remarks:
Reference: MITI, Japan

*2.4 VAPOUR PRESSURE

Value: 3.3 x 10^{-4} Pa
Temperature: 25 °C
Method: calculated [ ], measured [ X ]
OECD TG 104
GLP: Yes [ X ] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks:
Reference: MITI, Japan.

*2.5 PARTITION COEFFICIENT log_{10}P_{ow}

Log Pow: 3.5
Temperature: 25 °C
Method: calculated [ ]; measured [ X ]
OECD TG 107 HPLC method
GLP: Yes [ X ] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks:
Reference: MITI, Japan

*2.6 WATER SOLUBILITY

A. Solubility

Value: 0.15 mg/l
Temperature: 25 °C
Description: Miscible [ ]; Of very high solubility [ ]; Soluble [ ]; Slightly soluble [ ]; Of low solubility [ ]; Of very low solubility [ ]; Not soluble [ ]
Method: OECD TG 105
GLP: Yes [ X ] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks:
Reference: MITI, Japan

B. pH Value, pKa Value

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 STABILITY

*3.1.2 STABILITY IN WATER

Type: Abiotic (hydrolysis) [ X ]; biotic (sediment)[ ]
Half life: Stable in pH 4 at 25 °C
65.9 days in pH 7 at 25 °C
1.04 days in pH 9 at °C
Method: OECD TG 111
GLP: Yes [ X ] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks:
Reference: MITI, Japan

*3.2 MONITORING DATA (ENVIRONMENTAL)

No studies located

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION

*3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)
### Media:
- Air-biota
- Air-biota-sediment-soil-water
- Water-air
- Water-biota
- Water-soil
- Other

### Method:
- Fugacity level I
- Fugacity level II
- Fugacity level III [X]
- Fugacity level IV
- Other (calculation)
- Other (measurement)

### Results:

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Release 100% to air</th>
<th>Release 100% to water</th>
<th>Release 100% to soil</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>11.6 %</td>
<td>0.7 %</td>
<td>0.0 %</td>
</tr>
<tr>
<td>Water</td>
<td>10.3 %</td>
<td>87.9 %</td>
<td>0.4 %</td>
</tr>
<tr>
<td>Soil</td>
<td>77.2 %</td>
<td>4.4 %</td>
<td>99.6 %</td>
</tr>
<tr>
<td>Sediment</td>
<td>0.8 %</td>
<td>7.1 %</td>
<td>0.0 %</td>
</tr>
</tbody>
</table>

### Remarks:
- Appendix 1

### Reference:
- MITI, Japan

### 3.5 BIODEGRADATION

- **Type:** aerobic [X]; anaerobic [ ]
- **Inoculum:** adapted [ ]; non-adapted [X];
- **Concentration of the chemical:** related to COD [ ]; DOC [ ]; test substance [X]
- **Medium:** water [X]; water-sediment [ ]; soil [ ]; sewage treatment [ ]
- **Degradation:** 6 % by BOD after 28 days
- 7 % by HPLC after 28 days

### Results:
- readily biodeg. [ ]; inherently biodeg. [ ]; under test condition no biodegradation observed [X], other [ ]

### Method:
- OECD TG 301C

### GLP:
- Yes [X] No [ ] ? [ ]

### Test substance:
- purity: 99.9 %

### Remarks:
- partially degraded to carboxylic acid and methanol

### Reference:
- MITI, Japan

### 3.7 BIOACCUMULATION

- **Species:** Carp (*Cyprinus carpio*)
- **Exposure period:** 6 weeks
- **Temperature:** 25 °C
- **Concentration:**
  1. 0.1 mg/L
  2. 0.01 mg/L
- **BCF:**
  1. 6.1 – 63
  2. 7.1 – 23

### Method:
- OECD TG 305C

### Type of test:
- calculated [ ]; measured [X]
- static [ ]; semi-static [ ]; flow-through [X]; other (*e.g. field test*) [ ]

### GLP:
- Yes [X] No [ ] ? [ ]

### Test substance:
- purity: 99.9 %

### Remarks:

### Reference:
- MITI, Japan
4. **ECOTOXICITY**

*4.1 ACUTE/PROLONGED TOXICITY TO FISH*

(a) **Type of test:** static [ ]; semi-static [ X ]; flow-through [ ]; other (*e.g. field test*) [ ]
open-system [ X ]; closed-system [ ]

**Species:** *Oryzias latipes* (Himedaka)

**Exposure period:** 96 h

**Results:** $LC_{50}$ (96h) > 0.1 mg/l

**Analytical monitoring:** Yes [ X ] No [ ] ? [ ]

**Method:** OECD TG 203 (1992)

**GLP:** Yes [ X ] No [ ] ? [ ]

**Test substance:** As prescribed by 1.1 - 1.4, purity: 99.91 %

**Remarks:** Group of 10 Himedaka were exposed to measured concentration of 0.1 mg/l*, solubilizer (tetrahydrofuran (THF) 8.0 mg/l, hydrogenated castor oil (HCO-30) 92.0 mg/l) control and laboratory water control (dechlorinated tapwater). The $LC_{50}$ (96h).

* 0.1 mg/l is the highest concentration that DND could be dispersed.

**Reference:** Environment Agency of Japan (1996)

(b) **Type of test:** static [ ]; semi-static [ ]; flow-through [ X ]; other (*e.g. field test*) [ ]
open-system [ X ]; closed-system [ ]

**Species:** *Oryzias latipes* (Himedaka)

**Exposure period:** 14 d

**Results:** $LC_{50}$ (14d) > 0.1 mg/l

**Analytical monitoring:** Yes [ X ] No [ ] ? [ ]

**Method:** OECD TG 203 (1992)

**GLP:** Yes [ X ] No [ ] ? [ ]

**Test substance:** As prescribed by 1.1 - 1.4, purity: 99.91 %

**Remarks:** Group of 10 Himedaka were exposed to measured concentration of 0.1 mg/l*, solubilizer (THF 8.0 mg/l, HCO-30 92.0 mg/l) control and laboratory water control.

* 0.1 mg/l is the highest concentration that DND could be dispersed.

**Reference:** Environment Agency of Japan (1996)

4.2 **ACUTE TOXICITY TO AQUATIC INVERTEBRATES**

*A. Daphnia*

**Type of test:** static [ ]; semi-static [ X ]; flow-through [ ]; other (*e.g. field test*) [ ]
open-system [ X ]; closed-system [ ]

**Species:** *Daphnia Magna.*

**Exposure period:** 48 h
Results: EC$_{50}$ (48h) > 0.1 mg/l
Analytical monitoring: Yes [X] No [ ] ? [ ]
Method: OECD TG 202
GLP: Yes [X] No [ ] ? [ ]
Test substance: As prescribed by 1.1 - 1.4, purity: 99.91%
Remarks: 20 daphnids (4 replicates; 5 organisms per replicate) were exposed to measured concentration of 0.1 mg/l*, solubilizer (THF 8.0 mg/l, HCO$_3^-$ 92.0 mg/l) control and laboratory water control.
* 0.1 mg/l is the highest concentration that DND could be dispersed.


4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

Species: *Selenastrum capricornutum* ATCC 22662
Endpoint: Biomass [X]; Growth rate [ ]; Other [ ]
Exposure period: 72 h
Results: Biomass EC$_{50}$ (72h) > 0.1 mg/l
(Endpoint) NOEC > 0.1 mg/l
Analytical monitoring: Yes [X] No [ ] ? [ ]
open-system [ ]; closed-system [X]
GLP: Yes [X] No [ ] ? [ ]
Test substance: As prescribed by 1.1 - 1.4, purity: 99.91%
Remarks: Static test. The EC$_{50}$ value for biomass was calculated based on measured concentration (0.1 mg/l*). THF (4.0 mg/l) and HCO-30 (96.0 mg/l) was used as solubilizer.
* 0.1 mg/l is the highest concentration that DND could be dispersed.


4.4 TOXICITY TO BACTERIA

No data

4.5 CHRONIC TOXICITY TO AQUATIC ORGANISMS

No data

4.5.1 CHRONIC TOXICITY TO FISH

(*) 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type of test: static [ ]; semi-static [X]; flow-through [ ]; other (*e.g. field test*) [ ]; open-system [X]; closed-system [ ]
Species: *Daphnia Magna*
Endpoint: Mortality [ ]; Reproduction rate [X]; Other [X]
Exposure period: 21 d
Results: Reproduction rate: EC$_{50}$ (21 d) > 0.02 mg/l (Endpoint) NOEC > 0.02 mg/l

Analytical monitoring: Yes [ X ] No [ ] ? [ ]


GLP: Yes [ X ] No [ ] ? [ ]

Test substance: As prescribed by 1.1 - 1.4, purity: 99.91 %

Remarks: Forty daphnids (4 replicates; 10 daphnids per replicate) were exposed to nominal concentration of 0.02* mg/l (measured concentration; 0.018 mg/l at the start of exposure, 0.007 and < 0.001 mg/l after 1 and 2 days, respectively), solubilizer control (THF, 1.6 mg/l and HCO-50, 28.4 mg/l) or laboratory water control (dechlorinated tap water). The test water was renewed with 2 or 3 d cycles.

* 0.02 mg/l is the highest concentration that DND could be dispersed.


4.6 TOXICITY TO TERRESTRIAL ORGANISMS

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

No data

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

No data

4.6.3 TOXICITY TO OTHER NON MAMMALIAN TERRESTRIAL SPECIES (INCLUDING AVIAN)

No data

4.7 BIOLOGICAL EFFECTS MONITORING (INCLUDING BIOMAGNIFICATION)

No data

4.8 BIOTRANSFORMATION AND KINETICS

No data

4.9 ADDITIONAL REMARKS

None

5. TOXICITY

5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY
OECD SIDS DIMETHYL 2,6-NAPHTHALENEDICARBOXYLATE

Type: LD$_0$ [ ]; LD$_{100}$ [ ]; LD$_{50}$ [X]; LDL$_0$ [ ]; Other [ ]
Species/strain: Rat/Cj; CD (SD)
Value: >2,000 mg/kg b.w. for male and female
Discriminating dose: 0, 500, 1,000 and 2,000 mg/kg
Method: OECD TG 401
GLP: Yes [X] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks: No toxicity
Reference: MHW, Japan: 1997

5.1.2 ACUTE INHALATION TOXICITY
No available data

5.1.3 ACUTE DERMAL TOXICITY
No available data

5.1.4 ACUTE TOXICITY, OTHER ROUTES OF ADMINISTRATION
No available data

5.2 CORROSIVENESS/IRRITATION

5.2.1 SKIN IRRITATION/CORROSION
No available data

5.2.2 EYE IRRITATION/CORROSION
No available data

5.3 SKIN SENSITISATION
No available data

*5.4 REPEATED DOSE TOXICITY (SIDS data)
Species/strain: Rats/Crj; CD (SD)
Sex: Female [ ]; Male [ ]; Male/Female [X]; No data [ ]
Route of Administration: Oral (by gavage)
Exposure period: Males; 49 days,
Females; from 14 days before mating to day 3 of lactation
Frequency of treatment: Daily
Post exposure observation period:
Dose: 30, 100, 300, 1,000 mg/kg/day (in 0.5 % Na-CMC)
Control group: Yes [X]; No [ ]; No data [ ];
Concurrent no treatment[ ]; Concurrent vehicle [X]; Historical[ ]
NOAEL: Male: 1,000 mg/kg/day
Female: 1,000 mg/kg/day
Results: Any toxicological effects were not observed.

Method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test

GLP: Yes [X] No [ ] ? [ ]

Test substance: purity: 99.9 %

Reference: MHW, Japan: 1997

*5.5 GENETIC TOXICITY IN VITRO

A. BACTERIAL TEST

Type: Bacterial reverse mutation assay

System of testing: Salmonella typhimurium TA100, TA1535, TA98, TA1537

Escherichia coli WP2 uvrA

Concentration: -S9: 0, 313, 625, 1250, 2500, 5000 µg/plate

+S9: 0, 313, 625, 1250, 2500, 5000 µg/plate

Metabolic activation: With [ ]; Without [ ]; With and Without [X]; No data [ ]

S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone.

Results:

Cytotoxicity conc: Toxicity was not observed at 5000 µg/plate in five strains with or without an S9 mix.

Precipitation conc: + ? -

Genotoxic effects: With metabolic activation: [ ] [ ] [X]

Without metabolic activation: [ ] [ ] [X]

Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD TG (471 and 472)

GLP: Yes [X] No [ ] ? [ ]

Test substance: purity: 99.9 %

Remarks:

Reference: MHW, Japan: 1997

NON-BACTERIAL IN VITRO TEST

Type: Chromosomal aberration test

System of testing: CHL/IU cell

Concentration: -S9 (continuous treatment): 0, 0.60, 1.2, 2.4 mg/ml

-S9 (short-term treatment): 0, 0.60, 1.2, 2.4 mg/ml

+S9 (short-term treatment): 0, 0.60, 1.2, 2.4 mg/ml

Metabolic activation: With [ ]; Without [ ]; With and Without [X]; No data [ ]

S9: Rat liver, induced with phenobarbital and 5,6-benzoflavone.

Results:

Cytotoxicity conc: clastogenicity polyploidy + ? - + ? -

Genotoxic effects: With metabolic activation: [ ] [ ] [X] [ ] [ ] [X]

Without metabolic activation: [ ] [ ] [X] [ ] [ ] [X]
Method: Guidelines for Screening Mutagenicity Testing of Chemicals (Japan) and OECD TG (473).
GLP: Yes [X] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks: Structural chromosomal aberrations were not induced in any treatment group. With continuous treatment for 48 h, polyploidy (1.25%) was weakly induced at 2.4 mg/ml (high concentration).
Reference: MHW, Japan: 1997

* 5.6 GENETIC TOXICITY IN VIVO

No available data

5.7 CARCINOGENICITY

No available data

*5.8 TOXICITY TO REPRODUCTION

Type: Fertility [ ]; One-generation study [ ]; Two-generation study [ ]; Other [X]
Species/strain: Rats/Crj: CD (SD)
Sex: Female [ ]; Male [ ]; Male/Female [X]; No data [ ]
Route of Administration: Oral (gavage)
Exposure period: Male: For 2 weeks prior to mating and 2 weeks of mating
Female: For 2 weeks prior to mating, 2 weeks of mating and throughout pregnancy until day 3 postpartum
Frequency of treatment: Daily
Post exposure observation period:
Premating exposure period: male: 14 days, female: 14 days
Duration of the test:
Dose: 30, 100, 300, 1,000 mg/kg/day (in 0.5 % Na-CMC)
Control group: Yes [X]; No [ ]; No data [ ]; Concurrent no treatment [ ]; Concurrent vehicle [X]; Historical [ ]
NOAEL Parental: Male: 1,000 mg/kg, Female: 1,000 mg/kg
NOAEL F1 Offspring: 1,000 mg/kg
Results: Any toxicity was not observed.
Method: OECD Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
GLP: Yes [X] No [ ] ? [ ]
Test substance: purity: 99.9 %
Remarks:
Reference: MHW, Japan: 1997

*5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

No available data

5.10 OTHER RELEVANT INFORMATION
A. Specific toxicities

No available data

B. Toxicodynamics, toxicokinetics

No available data

* 5.11 EXPERIENCE WITH HUMAN EXPOSURE

No available data

6. REFERENCES

### Appendix 1

#### Scenario 1

<table>
<thead>
<tr>
<th></th>
<th>Emission Rate [kg/h]</th>
<th>Concentration [g/m³]</th>
<th>Amount [kg]</th>
<th>Percent [%]</th>
<th>Transformation Rate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>1,000</td>
<td>7.1.E-06</td>
<td>7.1.E+04</td>
<td>11.6</td>
<td>1.8.E+02</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>3.2.E-03</td>
<td>6.3.E+04</td>
<td>10.3</td>
<td>5.1.E+00</td>
</tr>
<tr>
<td>Soil</td>
<td>0</td>
<td>3.0.E-01</td>
<td>4.7.E+05</td>
<td>77.2</td>
<td>3.8.E+01</td>
</tr>
<tr>
<td>Sediment</td>
<td>5.1.E-02</td>
<td>5.1.E+03</td>
<td>0.8</td>
<td></td>
<td>4.1.E-01</td>
</tr>
<tr>
<td>Total Amount</td>
<td>6.1.E+06</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Scenario 2

<table>
<thead>
<tr>
<th></th>
<th>Emission Rate [kg/h]</th>
<th>Concentration [g/m³]</th>
<th>Amount [kg]</th>
<th>Percent [%]</th>
<th>Transformation Rate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0</td>
<td>6.3.E-07</td>
<td>6.3.E+03</td>
<td>0.7</td>
<td>1.6.E+01</td>
</tr>
<tr>
<td>Water</td>
<td>1000</td>
<td>4.2.E-02</td>
<td>8.4.E+05</td>
<td>87.9</td>
<td>6.8.E+01</td>
</tr>
<tr>
<td>Soil</td>
<td>0</td>
<td>2.6.E-02</td>
<td>4.2.E+04</td>
<td>4.4</td>
<td>3.4.E+00</td>
</tr>
<tr>
<td>Sediment</td>
<td>6.8.E-01</td>
<td>6.8.E+04</td>
<td>7.1</td>
<td></td>
<td>5.4.E+00</td>
</tr>
<tr>
<td>Total Amount</td>
<td>9.6.E+05</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Scenario 3

<table>
<thead>
<tr>
<th></th>
<th>Emission Rate [kg/h]</th>
<th>Concentration [g/m³]</th>
<th>Amount [kg]</th>
<th>Percent [%]</th>
<th>Transformation Rate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0</td>
<td>1.2.E-07</td>
<td>1.2.E+03</td>
<td>0.0</td>
<td>3.2.E+00</td>
</tr>
<tr>
<td>Water</td>
<td>0</td>
<td>2.1.E-03</td>
<td>4.1.E+04</td>
<td>0.4</td>
<td>3.3.E+00</td>
</tr>
<tr>
<td>Soil</td>
<td>1000</td>
<td>7.3.E+00</td>
<td>1.2.E-07</td>
<td>99.6</td>
<td>9.4.E+02</td>
</tr>
<tr>
<td>Sediment</td>
<td>3.3.E-02</td>
<td>3.3.E+03</td>
<td>0.0</td>
<td></td>
<td>2.7.E-01</td>
</tr>
<tr>
<td>Total Amount</td>
<td>1.2.E+07</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Scenario 4

<table>
<thead>
<tr>
<th></th>
<th>Emission Rate [kg/h]</th>
<th>Concentration [g/m³]</th>
<th>Amount [kg]</th>
<th>Percent [%]</th>
<th>Transformation Rate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>600</td>
<td>4.5.E-06</td>
<td>4.5.E+04</td>
<td>2.4</td>
<td>1.1.E+02</td>
</tr>
<tr>
<td>Water</td>
<td>300</td>
<td>1.5.E-02</td>
<td>3.0.E+05</td>
<td>16.1</td>
<td>2.4.E+01</td>
</tr>
<tr>
<td>Soil</td>
<td>100</td>
<td>9.2.E-01</td>
<td>1.5.E+06</td>
<td>80.2</td>
<td>1.2.E+02</td>
</tr>
<tr>
<td>Sediment</td>
<td>2.4.E-01</td>
<td>2.4.E+04</td>
<td>1.3</td>
<td></td>
<td>1.9.E-00</td>
</tr>
<tr>
<td>Total Amount</td>
<td>1.8.E+06</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Physico-chemical parameter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Method</th>
<th>Temp. [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>244.25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>199.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapor pressure [Pa]</td>
<td>3.30E-04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water solubility [g/m³]</td>
<td>0.15</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Log Kow</td>
<td>3.5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Half life [h]</td>
<td>in air</td>
<td>272</td>
<td>Estimated</td>
<td></td>
</tr>
<tr>
<td></td>
<td>in water</td>
<td>8640</td>
<td>Estimated</td>
<td></td>
</tr>
<tr>
<td></td>
<td>in soil</td>
<td>8640</td>
<td>Estimated</td>
<td></td>
</tr>
</tbody>
</table>

### Environmental parameter

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Volume [m³]</th>
<th>Depth [m]</th>
<th>Area [m²]</th>
<th>Organic carbon [%]</th>
<th>Lipid content [mg/g]</th>
<th>Density [kg/m³]</th>
<th>Residence [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk air</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air particles</td>
<td>2.0E+03</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.0E+13</td>
<td>1000</td>
<td>1E+10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk water</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water particles</td>
<td>1.0E+06</td>
<td></td>
<td></td>
<td>0.04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fish</td>
<td>2.0E+05</td>
<td></td>
<td></td>
<td>0.05</td>
<td>1000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>2.0E+10</td>
<td>1000</td>
<td>2E+09</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk soil</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>3.2E+08</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>4.8E+08</td>
<td></td>
<td></td>
<td></td>
<td>1000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid</td>
<td>8.0E+08</td>
<td></td>
<td></td>
<td>0.04</td>
<td>2400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>1.6E+09</td>
<td>0.2</td>
<td>8E+09</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk sediment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>8.0E+07</td>
<td></td>
<td></td>
<td></td>
<td>1000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solid</td>
<td>2.0E+07</td>
<td></td>
<td></td>
<td>0.06</td>
<td>2400</td>
<td>50000</td>
<td></td>
</tr>
</tbody>
</table>

### Intermedia Transport Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>m/h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air side air-water MTC</td>
<td>5</td>
</tr>
<tr>
<td>Water side air water MTC</td>
<td>0.05</td>
</tr>
<tr>
<td>Rain rate</td>
<td>1E-04</td>
</tr>
<tr>
<td>Aerosol deposition</td>
<td>6E-10</td>
</tr>
<tr>
<td>Soil air phase diffusion MTC</td>
<td>0.02</td>
</tr>
<tr>
<td>Soil water phase diffusion MTC</td>
<td>1E-05</td>
</tr>
</tbody>
</table>

---

**OECD SIDS**

**DIMETHYL 2,6-NAPHTHALENEDICARBOXYLATE**

**UNEP Publications**