

본 자료는 “화학물질등록평가법 시행령 제13조 및 같은법 시행규칙 제5조”에 따라 제출이 필요한 생략사유 및 증명자료의 예시로 공개하는 자료입니다. 해당 자료의 내용 및 양식은 추가검토·보완을 통해 수정·변경될 수 있습니다.

## 예시 1

### 국가·국제기구 평가보고서를 통한 시험항목의 자료제출 생략사유 및 증명자료

대상물질 : Dichlorodimethylstannane(CAS No. 753-73-1)

시험항목 : pH에 따른 가수분해

#### 등록제출자료 생략의 사유

**(출처명)** 본 생략사유 및 증명자료는 OECD SIDS 초기평가 보고서(SIAR: SIDS Initial Assessment Report for 23<sup>th</sup> SIAM, 2006) 결과를 참고하였습니다.

**(주요 종말점 및 결과값과 주요영향)** Dichlorodimethylstannane(CAS No. 753-73-1)의 pH에 따른 가수분해 반감기( $t_{1/2}$ ) 값은 > 1년(pH 4, 7, 9)(GLP)으로 기술되어 있습니다.

**(생략 시험항목)** 해당결과를 통해 pH에 따른 가수분해를 판단할 수 있으므로 화학물질의 등록 및 평가 등에 관한 법률 시행령 제13조 제6호의2에 따라 Dichlorodimethylstannane(CAS No. 753-73-1)의 pH에 따른 가수분해 자료를 생략하고자 합니다.

#### 증명자료

생략사유의 증명자료로 아래와 같이 해당자료의 국문요약을 참고로 제시합니다.

#### <표> pH에 따른 가수분해 시험결과(요약)

출처: SIDS Initial Assessment Report for 23th SIAM(2006), 34~37쪽

No.	자료개요 및 시험방법	시험결과
1	<ul style="list-style-type: none"><li>- 자료의 성격: 주요자료, 요약서</li><li>- 신뢰도: 신뢰도 2 (제한적인 신뢰도)</li><li>- 근거(인용): OECD SIAR 보고서 급성독성 평가 자료</li><li>- 시험방법: OECD Guide-line 111</li><li>- GLP 준수여부: GLP 준수</li><li>- 시험물질 정보: Dichlorodimethylstannane(순도: 99.66%)</li><li>- 농도분석: sodium tetraethylborate (STEB)로 유도체화 시킨 후 hexane으로 추출하여 GC/MS 분석함</li></ul>	<ul style="list-style-type: none"><li>- 결과값 :<ul style="list-style-type: none"><li>• <math>t_{1/2}</math> (pH 4): &gt;1년 (25 °C)</li><li>• <math>t_{1/2}</math> (pH 7): &gt;1년 (25 °C)</li><li>• <math>t_{1/2}</math> (pH 9): &gt;1년 (25 °C)</li></ul></li></ul>

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[별첨(원문 페이지 발췌)]

시험결과 표(또는 내용)

### 3. Environmental Fate and Pathways

Id 753-73-1

Date 24.07.2006

water. This deviation did not affect the validity of the results of the study.

GLP: yes

STATISTICAL METHODS: None.

METHOD OF CALCULATION: The percentage hydrolysis was calculated as:  $[(\text{mean concentration (mg DMT/l)} \text{ at } t=5 \text{ days} - \text{mean concentration (mg DMT/l)} \text{ at } t=0) / (\text{mean concentration (mg DMT/l)} \text{ at } t=0)] * 100\%$ .

ANALYTICAL METHODS: All test substance solutions (in buffer solutions and Milli-Q water) were derivatised with sodium tetraethylborate (STEB), extracted with hexane and analysed with GC-MS.

Principle of the analytical method: An aliquot of an internal standard solution (containing tetrapropyltin, tripropyltin chloride, diheptyltin dichloride and monoheptyltin trichloride) was added to all samples of the test material. Acetate buffer solution pH 4.5, STEB reagent (20% (m/V)) and hexane were added and mixed. In this way, the organotin compounds were converted to their corresponding ethylated derivatives and extracted into the hexane layer. The hexane added also contained naphthalene as an internal standard to check the injection of sample into the GC-MS. The derivatisation and extraction were carried out simultaneously. The hexane solutions containing the derivatised organotin compounds were extracted with 2 mol/l HCl in order to remove any ethylboron compounds present, which might interfere with the GC-MS analysis. The DMT concentration in water was determined by GC-MS analysis of hexane extracts.

OTHER: The purpose of the study was to determine the percentage hydrolysis of the substance in aqueous solutions after 5 days at 50°C at pH values of 4.0, 7.0 and 9.0.

#### Result

#### : TEST SUBSTANCE CONCENTRATION:

- Actual substance concentration in buffer solutions: The recovery of the substance in buffer solutions pH 4.0, pH 7.0, and pH 9.0, and in Milli-Q water were 96%, 99%, 94% and 97%, respectively. The blank buffer solutions and Milli-Q water did not show peak concentrations for the substance (i.e. concentrations were <1 mg/l).

- Actual substance concentration in QC samples: The recovery of the QC samples of the substance in buffer solutions pH 4.0, pH 7.0, and pH 9.0, and Milli-Q water, were between the required 80-120% of the prepared concentrations (ranged from 96-107% of the prepared concentrations).

#### CONTROLS:

- Calibration graphs: All calibration graphs used for determination of the concentration of the substance in validation samples and in hydrolysis solutions were linear, i.e., the correlation coefficient  $r$  obtained after linear regression of the calibration graphs constructed from the organotin calibration solutions (Q-value (ratio peak area test substance / peak area internal standard) vs. concentration) was at least 0.99. Calibration graphs of the substance in Milli-Q water:  $r > 0.998$ .

- Biodegradation: The sterility tests performed at the end of the hydrolysis tests did not show any bacterial activity. Biodegradation of the test substance in the hydrolysis solutions did not occur.

#### HYDROLYSIS:

- Actual pH of the hydrolysis solutions: The pH of the substance in the pH 4.0 buffer solution was 4.01, 4.03 and 4.05, respectively on  $t=0$ ,  $t=1$  day and  $t=5$  days. The pH of the substance in the pH 7.0 buffer solution was 7.02, 7.04 and 7.05, respectively on  $t=0$ ,  $t=1$  day and  $t=5$  days. The pH of the substance in the pH 9.0 buffer solution was 8.98, 8.99 and 8.96, respectively on  $t=0$ ,  $t=1$  day and  $t=5$  days. The pH of the substance in Milli-Q water was 3.47, 3.44 and 3.56, respectively on  $t=0$ ,  $t=1$  day and  $t=5$  days. All pH values remained within  $\pm 0.1$  of the initial pH values.

- Hydrolysis % (pH 4.0): The mean measured concentrations (in mg/l) of the substance in hydrolysis solution pH 4.0 were 103.2, 100.5 and 95.4 on  $t=0$ ,  $t=1$  day and  $t=5$  days, respectively. The relative difference between the concentration at  $t=5$  days and  $t=0$  was -7.6%.

- Hydrolysis % (pH 7.0): The mean measured concentrations (in mg/l) of the substance in hydrolysis solution pH 7.0 were 100.7, 105.0 and 102.9 on  $t=0$ ,

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#### Result

A second experiment was conducted, in order to simulate exposure to natural light (i.e., light wavelengths >290 nm). This experiment was only conducted qualitatively; breakdown products were identified but not quantified. The same apparatus as in the first experiment was used to irradiate the methyltin chloride solutions; however, a glass plate was placed between the source and the solution cells to block all light wavelengths <300 nm.

: The pH of the 0.05 M test solutions of TMTC, DMTC, and MMTC were measured as 3.6, 2.4, and 1.4, respectively.

Maximum UV absorbance wavelength, by test substance:

TMTC: 208 nm (single peak)

DMTC: 203 and 228 nm (two distinct peaks)

MMTC: 220 nm (single, broad band)

Based on these absorbance maximums, irradiation with wavelengths >235 nm would be expected to cause breakdown at a much slower rate.

During irradiation, a fine white particulate appeared in all test solutions. Elemental and Mössbauer analyses determined that the precipitate was hydrated tin dioxide (SnO<sub>2</sub>). Approximately 60 hours of irradiation reduced the TMTC solution to 50% of the original concentration (i.e., 0.025 M), while DMTC was reduced to 20% of the original concentration after 110 hours (50% degradation was estimated to require 300 hours). MMTC degraded at an even slower rate, which was not quantified due to the excessive irradiation time required. However, the SnO<sub>2</sub> precipitate occurred after 30 hours, while in the DMTC solution only 6 hours was required. The author concluded that the breakdown of MMTC could be estimated as 5 times slower than DMTC (i.e., 50% degradation after 1500 hours).

Qualitative results of the second experiment indicated that irradiation with light wavelengths >300 nm (i.e., natural light) produced the same degradation products, although at a slower rate.

#### Source

#### Test substance

#### Reliability

18.08.2004

Study results indicate that methyltin chloride compounds in water, irradiated with UV light, degrade to form inorganic tin compounds.

: Blunden. 1983

: Dimethyltin Dichloride [CAS No. 753-73-1]; purity/source not reported.

: (2) valid with restrictions

Non-guideline study; meets generally-accepted scientific standards.

(18)

#### 3.1.2 STABILITY IN WATER

#### Type

: abiotic

#### t1/2 pH4

: > 1 year at 25 °C

#### t1/2 pH7

: > 1 year at 25 °C

#### t1/2 pH9

: > 1 year at 25 °C

#### Deg. product

: no

#### Method

: OECD Guide-line 111 "Hydrolysis as a Function of pH"

#### Year

: 2002

#### GLP

: yes

#### Test substance

: other TS

#### Method

: METHOD FOLLOWED: OECD Guidelines for the testing of chemicals, proposal for updating guideline 111, revised guideline 111 (2002).  
DEVIATIONS FROM GUIDELINE: Simultaneous with the preliminary hydrolysis tests in buffer solutions at pH 4.0, 7.0 and 9.0, a hydrolysis experiment of dichlorodimethylstannane was also carried out in Milli-Q