

I U C L I D

Data Set

Existing Chemical : ID: 26140-60-3
CAS No. : 26140-60-3
EINECS Name : terphenyl
EC No. : 247-477-3
TSCA Name : Terphenyl, Mixed
Molecular Formula : C18H14

Producer related part
Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part
Company : Solutia Inc.
Creation date : 17.03.2003

Status :
Memo :

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Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

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2.1 MELTING POINT

Value : 76 - °C
Sublimation :
Method : other: Internal assay
Year : 1983
GLP : no
Test substance : other TS

Remark : Beginning of slurry point with range of 76-80 deg. C.
Test substance : THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 % Quaterphenyls and 4 % High Boilers

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003 (1)

Value : 145 - °C
Sublimation :
Method : other: Monsanto internal assay
Year : 1980
GLP : no
Test substance : other TS

Remark : Pour point
Test substance : Santowax R consisting of 81% Mixed Terphenyls, 17% Quaterphenyls and 2% High Boilers.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003 (2)

Value : = 210.1 - °C
Sublimation :
Method : other: calculated (MPBPWIN v1.40)
Year : 2003
GLP : no
Test substance : other TS

Test substance : Terphenyl [CAS No. 26140-60-3]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003 (3)

2.2 BOILING POINT

Value : 343 - °C at
Decomposition :
Method : other: Internal assay
Year : 1983
GLP : no
Test substance : other TS

Test substance : THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 % Quaterphenyls and 4 % High Boilers

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003 (1)

2. Physico-Chemical Data

Id 26140-60-3
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Value	:	364 - °C at	
Decomposition	:		
Method	:	other: Internal assay	
Year	:	1980	
GLP	:	no	
Test substance	:	other TS	
Test substance	:	SANTOWAX R consisting of 82 % Mixed Terphenyls, 16 % Quaterphenyls and 2 % High Boilers.	
Reliability	:	(2) valid with restrictions	
Flag	:	Critical study for SIDS endpoint	
09.07.2003			(4)
Value	:	= 376 - °C at	
Decomposition	:		
Method	:	other: calculated (MPBPWIN v1.40)	
Year	:	2003	
GLP	:	no	
Test substance	:	other TS	
Test substance	:	Terphenyl [CAS No. 26140-60-3]	
Reliability	:	(2) valid with restrictions	
09.07.2003			(3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.0000081 - hPa at 25 °C	
Decomposition	:		
Method	:	other (measured)	
Year	:	1982	
GLP	:	no data	
Test substance	:	other TS	
Method	:	Internal technical analysis	
Test substance	:	THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 % Quaterphenyls and 4 % High Boilers	
Reliability	:	(2) valid with restrictions	
Flag	:	Critical study for SIDS endpoint	
09.07.2003			(5)
Value	:	= .00000412 - hPa at 25 °C	
Decomposition	:		
Method	:	other (calculated)	
Year	:	1985	
GLP	:	no	
Test substance	:	other TS	
Remark	:	Reported as 3.09 x 10e-6 mm Hg @ 25 deg. C	
Test substance	:	Terphenyl [CAS No. 26140-60-3]	
Reliability	:	(2) valid with restrictions	
09.07.2003			(6)

2.5 PARTITION COEFFICIENT

Partition coefficient	: octanol-water	
Log pow	: = 6.03 - at °C	
pH value	: -	
Method	: other (measured): not reported	
Year	: 1993	
GLP	: no data	
Test substance	: other TS	
Test substance	: Therminol 75 consisting of 62% Mixed (2% ortho-, 55% meta-, 5 % para-) Terphenyls, 34 % Quaterphenyls and 4 % High Boilers.	
Reliability	: (2) valid with restrictions	
Flag	: Critical study for SIDS endpoint	
09.07.2003		(7)
Partition coefficient	: octanol-water	
Log pow	: 5.16 - at °C	
pH value	: -	
Method	: other (calculated)	
Year	: 1990	
GLP	:	
Test substance	: other TS	
Method	: Calculated method using equation $\text{Log Kow} = 5.00 - 0.67$ (log water solubility), based on Chiou et al 1977.	
Test substance	: THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 % Quaterphenyls and 4 % High Boilers	
Reliability	: (2) valid with restrictions	
09.07.2003		(8)
Partition coefficient	: octanol-water	
Log pow	: 5.21 - at °C	
pH value	: -	
Method	: other (calculated)	
Year	: 1990	
GLP	:	
Test substance	: other TS	
Method	: Calculated method using equation $\text{Log Kow} = 5.00 - 0.67$ (log water solubility), based on Chiou et al 1977.	
Test substance	: Santowax R consisting of 81% Mixed Terphenyls, 17% Quaterphenyls and 2% High Boilers.	
Reliability	: (2) valid with restrictions	
09.07.2003		(8)
Partition coefficient	: octanol-water	
Log pow	: = 5.52 - at °C	
pH value	: -	
Method	: other (calculated): atom/fragment contribution method	
Year	: 1995	
GLP	: no	
Test substance	: other TS	
Method	: Individual atom/fragment contribution (AFC) values were determined for 130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and correction factors for a given chemical structure.	
Test substance	: Terphenyl [CAS No. 26140-60-3]	
Reliability	: (2) valid with restrictions	

2. Physico-Chemical Data

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .151 mg/l at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year : 1982
GLP : no data
Test substance : other TS

Method : Measured, saturated column method. Test material was coated at the 5% level on 89/100 mesh Chromosorb WHP, which was then loaded into the saturator column. The concentration of test substance in the solution (test water was deionized MilliQ water) leaving the saturator column was measured using a coupled column LC technique fitted with a UV detector. Four separate runs were made varying flow through rate (1 or 2.3 mL/min) and total volume collected (either 5 or 10 mL).

Result : 0.151 +/- 0.013 mg/L at 25 deg. C.
Test substance : Test substance was MCS-1980 consisting of 61% Mixed Terphenyls, 34% Quaterphenyls, and approx. 4% High Boilers.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

23.06.2003

(10)

Solubility in : Water
Value : .11 mg/l at 23 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 1979
GLP : no
Test substance : other TS

Method : Presumed similar to methods used for MCS 1980.
Test substance : SANTOWAX R consisting of 82 % Mixed Terphenyls, 16 % Quarterphenyls and 2 % High Boilers.

Reliability : (2) valid with restrictions

09.07.2003

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Solubility in : Water
Value : = .215 - at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :

2. Physico-Chemical Data

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pKa : at 25 °C
Description : slightly soluble (0.1-100 mg/L)
Stable :
Deg. product :
Method : other: calculated
Year : 1996
GLP : no
Test substance : other TS

Method : Estimation performed using regression equations based on log Kow values.

Test substance : Terphenyl [CAS No. 26140-60-3].

Reliability : (2) valid with restrictions

09.07.2003

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2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : other
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Deg. product :
Method : other (calculated): AOPWIN v1.90
Year : 2003
GLP : no
Test substance : other TS

Remark : Vapor phase mixed terphenyls are susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as $9.1946E-12$ cm³/(molecule*sec). Based on $1.5E6$ OH molecules/cm³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 27.9 hours.

Test substance : Terphenyl [CAS No. 26140-60-3]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
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3.1.2 STABILITY IN WATER

Remark : The test substance (Terphenyl) is not susceptible to hydrolysis. It has only 3-membered aromatic rings associated with its structure, which are listed in Lyman in Table 7.1 - Types of Organic Functional Groups That Are Generally Resistant to Hydrolysis. Lyman, WJ, Reehl, WF and Rosenblatt, DH. 1990. Handbook of Chemical Property Estimation Methods. Environmental Behaviour of Organic Compounds. American Chemical Society, Washington, DC.

02.06.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air-water-soil-sediment
Air : 1.05 % (Fugacity Model Level I)
Water : 12 % (Fugacity Model Level I)
Soil : 43.8 % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : 43.1 % (Fugacity Model Level II/III)
Method : other

3. Environmental Fate and Pathways

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Year : 2003

Method : Used EPIWIN, Syracuse Research Corp. The following physical properties of Mixed Terphenyls were used as the model input parameters: water solubility=0.215 mg/L, vapor pressure = 3.09E-6 mm Hg; log Kow = 5.52; melting point = 210 Deg C. All property values were taken from this Robust Summary Dossier.

Remark : Air: half life = 27.9 hr; emissions = 1000 kg/hr
Water: half life = 900 hr; emissions = 1000 kg/hr
Soil: half life = 900 hr; emissions - 1000 kg/hr
Sediment: half life = 3600 hr; emissions - 0 kg/hr

Persistence Time: 993 hr

Test substance : Mixed Terphenyls
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : domestic sewage
Deg. product :
Method : other
Year : 1974
GLP : no
Test substance : other TS

Method : Semicontinuous activated sludge test. Twenty six (26) week test, 24-h cycle of draw and fill, weekly analyses of parent material using UV absorbance, while metabolites were quantified using GC -FID, 1 mg (week 1), 3 mg (week 2) and 5 mg (thereafter) of TS was added per cycle, activated sludge mixed liquor from municipal sewage treatment plant was inocula, a series of 3 hexane off gas scrubbers were used to catch volatiles.

Result : Overall mean daily disappearance rate was 11.5 +/- 7.2%. GC analyses showed that the several peaks that make up the TS degraded at varying levels. Analyses showed complete loss of o-terphenyl, a halving of m-terphenyl concentration, and little change in p-terphenyl concentration. No volatile losses were reported.

Test substance : THERMINOL 88, a mixture of 81% Mixed Terphenyls, 17 % Quaterphenyls and 2% Higher Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
02.06.2003

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Type : aerobic
Inoculum : domestic sewage
Deg. product :
Method : other: CO2 Shake Flask
Year : 1980
GLP : no
Test substance : other TS

3. Environmental Fate and Pathways

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- Method** : Used 50-day Shake Flask Ultimate Biodegradation study design. Two tests were performed, a 50-day test using an inoculum acclimated for 30 days. Test medium was a standard BOD medium enhanced with 2 times normal amount of phosphate buffer; 4 times normal amount of FeCL3, and 40 mg (NH4)2SO4 per liter purified water. Two liter triplicate flasks were fitted with barium hydroxide solution to catch CO2; glucose positive control, and then inoculum from acclimated solution were prepared using a 16 or 30 days SCAS procedure: activated aerated, suspended solids of 3000 mg/L, 24-h at the end of which it was settled for 30 min, 1L decanted, 1 L raw sewage added containing test substance. Initial bacterial counts in inoculum during SCAS preparation averaged 4.0E+6 and 3.1+6 CFU/ml. in the first and second tests respectively. Initial test substance was a nominal 20 mg/L. Analyzed using HPLC for test material remaining. Test vessels were incubated at 27+/- deg. C. in the dark on a rotary shaker.
- Result** : The positive control averaged approximately 100% thCO2. For the test using a 16-d inoculum, thCO2 formation averaged 7+/-3%. Chemical analyses at experiment end showed that only 4 to 55% of the initial test substance remaining in the first test and < 1 percent in the second test. Thus, primary degradation is relatively rapid, while the biodegradation products are more persistent.
- Test substance** : MCS 1980, which contained a mixture of 63% Mixed Terphenyls, 35% Quaterphenyls and 2% High Boilers.
- Reliability** : (2) valid with restrictions

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- Type** : aerobic
- Inoculum** :
- Contact time** : 7.5 month
- Degradation** : 94 - (±) % after 7.5 month
- Result** :
- Deg. product** :
- Method** : other: soil bacterial degradation
- Year** : 1988
- GLP** : no
- Test substance** : other TS

- Method** : Used a defined methodology to determine the degree of biodegradability caused by soil microorganisms from two separate soil samples. Two concentrations of test material (50 ppm and 0.5 ppm) were prepared in methylene chloride. Two soil types, (1) Missouri Bottoms, a sandy soil with 0.5% organic carbon and a moisture content of 11.3% at 1/3 BAR and (2) Florida muck, a heavy loam containing 32.9% organic carbon and an 82% moisture content at 1/3 BAR. Soil samples containing test material were analyzed by HPLC after 0, 0.5, 1, 2, 4, 6, 8, 12, 15, and 32 weeks on study. A microtox screen was employed prior to study start to insure no bacterial toxicity would interfere with the subsequent test. Method of detection of test material was validated on both soils prestudy. Soil samples were stabilized prior to study start such that they contained a uniform level of microorganisms. Soil samples (25 gm) were placed in 125 ml jars and spiked with 250 ul of test solution containing the test material in solvent. Jars were capped and shaken, then lids removed and restirred manually. After being lightly recapped, the jars containing the test material and soil were incubated in the dark at 25 deg. C and 80% humidity until sampled. Three replicates of each treated group plus a control per time period per soil type were used. Sterile controls and matrix blanks were also employed. Kinetic parameters were calculated from raw data.

- Remark** : Provided as Supplementary information.
- Result** : % Reduction Relative to Nominal Concentration after 32 Weeks on Test

Nominal Conc. % Red. Soil Type % Vs Sterile Soil T 1/2 (weeeks)

500 ppm 94 Mo. Bott. 81 8.1

3. Environmental Fate and Pathways

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500 ppm	94	Mo. Bott.	81	8.1
0.5 ppm	75	Mo. Bott.	-	16.0
500 ppm	84	Fla Muck	70	12.1
0.5 ppm	0	Fla Muck	-	no change

Terphenyl rapidly began to undergo biological degradation upon introduction to either sandy or loam soil types containing soil bacteria. Most of the loss observed was related to biological means although small differences in losses between untreated and sterile soil suggests some abiotic causes are also involved.

Test substance : Test substance labeled "Terphenyl" containing a mixture of terphenyl isomers.

Reliability : (2) valid with restrictions
09.07.2003

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3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : > - .75
LC50 : >= - .75
Method : other
Year : 1984
GLP : yes
Test substance : other TS

Method : Design based on USEPA (1975) 660/3-75-009 Committee on Methods for Toxicity Tests with Aquatic Organisms. Fathead minnows were obtained from inhouse cultures, held in tanks for 2 weeks under 16h light, 8h dark and fed commercial fish food until 48h before testing. Fish had a mean weight and length of 0.95 g and 45 mm, respectively. Static bioassay was performed in 20 L glass aquaria containing 15L of deionized reconstituted well water. Water quality of test dilution water at test initiation was: DO= 94-95% of saturation, pH=6.8-7.2, total hardness =28-34 mg/L CaCO₃, total alkalinity of 26-28 mg/L CaCO₃. Test water was maintained at 22 +/- 1 deg. C. in a water bath. Fish were held without food for 48 hr before testing and were not fed during the test. Nominal concentrations of 0.38, 0.75, 1.5 and 7.5 mg/L were prepared by adding test material to dimethylformamide. Test concentrations were not measured during the test. Test solutions were cloudy in all but the lowest concentration, signaling aqueous concentrations above the limit of solubility. Across all test vessels, DO ranged up to 8.6 mg/L, pH ranged between 6.7-7.5, and temperature ranged from 22-23 deg. C.

Result : Deaths of 0-20% were reported for all test levels at 96-h. The aqueous limit of solubility was estimated to be 0.75 mg/L. Since deaths ranged from 0 to 10% at the apparent limit of solubility the 96h LC50 value was considered to be => 0.75 mg/L. and the NOEC was > 0.75 mg/L.

Test substance : Therminol 75 which consisted of 62% Mixed Terphenyls, and 34% Quaterphenyls and 4% High Boilers.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

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Type : static
Species : Salmo gairdneri (Fish, estuary, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 27 - measured/nominal
Limit test : no
Analytical monitoring : no
Method : other
Year : 1979
GLP : yes
Test substance : other TS

Method : Used USEPA (1975) 660/3-75-009 Committee on Methods for Toxicity Test with Aquatic Organisms. Rainbow trout were obtained from a fish hatchery, held in culture tanks for 2 weeks under 16 h light, 8 hr dark. Fish were fed commercial fish food until 48 h before the test. Fish had a mean weight and length of 36 and 38.4 mm respectively, Static bioassays were performed in 5 gal glass vessels containing 15 L of laboratory well water, with 10 fish per concentration. Water quality of test dilution water at tes t

initiation: DO 8.9 mg/L, pH 7.8, total hardness 240 mg/l CaCO₃ total alkalinity 360 mg/L CaCO₃. Test water was maintained at 12 +/- 1 degree C in a water bath. Fish were held without food for 48 h before testing and were not fed during the test. Based on the results of a rangefinding test, test levels used were 5, 10, 21, 42, and 75 mg/L TS. Test material (yellow crystals) were mixed as a suspension in acetone, except in the two highest concentrations, which had Test Substance directly added to the water. Aliquots of the acetone suspension were added to the vessels to obtain the lower three nominal test concentrations. Water and TS were vigorously stirred. The compound was reported to precipitate and float in clumps in all test solutions, which is not surprising as the water solubility of this material is reportedly 0.15 mg/L. Actual test concentrations were not measured during the test. Across all test vessels DO ranged from 4.8-7.7 mg/L; pH ranged from 7.5 to 8.06; temperature remained at 12 degree C and ammonia remained below the toxic limit. LC50 and CI were calculated using the methods of Litchfield and Wilcoxon (J. Pharm. Exp. Ther 96: 99-113).

Remark	:	An initial test was also summarized in this study but has not been considered in this assessment as spurious, non dose-related deaths were observed in all test concentrations assayed. Thus, a second, repeat study has been summarized above. Provided as Supplemental information.	
Result	:	96-h LC50 = 27 mg/L (95% CI=20-37 mg/L). No control mortalities were reported. At 24-h no mortality was observed while at 48-h no mortalities were reported in the lower 3 concentrations with partial mortalities up to 50% in remaining concentrations. At 96-h, there were mortalities ranging from 0 - 100% in a dose related manner across all test concentrations.	
Test substance	:	THERMINOL 88, consisting of 82% Mixed Terphenyls, 16% Quaterphenyls and 2% High Boilers.	
Conclusion	:	No deaths were observed at levels of water saturation (low dose of 5 mg/L) which exceeded the water solubility. This HPV endpoint is considered complete, using a previous acute fish study in conjunction with the Chronic Fish robust summary cited in section 4.5.1.	
Reliability 19.06.2003	:	(2) valid with restrictions	(18)
Type	:		
Species	:	other: fish	
Exposure period	:	96 hour(s)	
Unit	:	mg/l	
LC50	:	= .028 -	
Method	:	other: calculated (EcoSAR)	
Year	:		
GLP	:	no	
Test substance	:	other TS	
Remark	:	An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR. Information supplied as Supplemental.	
Test substance 02.06.2003	:	Terphenyl [CAS No. 26140-60-3]	(19)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	< - .006
EC50	:	= - .043

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Method	: other
Year	: 1983
GLP	: yes
Test substance	: other TS
Method	: Used EPA method 660/3-75-009. 1975. Ten 24-h old <i>D. magna</i> Straus were tested at room temperature in a series of three replicates per test concentration. Test concentrations were 0.006, 0.012, 0.025, 0.05, 0.1 mg/mL, plus clean water and solvent (0.5 mL DMF) controls. Tests were conducted in well water from St Peters, MO. Test concentrations were not measured. Daphnids were not fed. Test vessels were not aerated. Tests were conducted in 250-mL beakers or jars containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured according to SOPs for dissolved oxygen, pH, alkalinity, hardness and temperature and no significant changes were observed in any parameter. During the 48-h test, pH ranged from 7.65 to 7.9, DO ranged from 7.8 to 8.1 mg/L. Temperature averaged 21deg. C., alkalinity ranged from 295-306 mg/L, and hardness ranged from 245 to 250 mg/L. The heavy metals and organochlorines that are routinely measured in the well water were presented in the appendices. At 48-h, there were 7% mortalities in the clean water and solvent controls. There were partial mortalities in a dose response fashion across all test concentrations. The estimated EC50 and 95% CI were determined using EPA statistical procedures.
Result	: 24-h EC50=>0.1 mg/L; 48-h EC50 (95%CL)=0.043 (0.029-0.074) mg/L.; NOEC<0.006 mg/L. % immobilized per dose level used (mg/L) after treatment (24-h:48-h)= control (0%:7%), solvent control (0:7), 0.006 (20:33), 0.012 (0:20), 0.025 (7:37), 0.05 (10:53), and 0.1 (13:70).
Test substance	: MCS 1980 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls and 4% High Boilers.
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
19.06.2003	(20)
Type	: static
Species	: <i>Daphnia magna</i> (Crustacea)
Exposure period	: 48 hour(s)
Unit	: mg/l
NOEC	: .056 -
EC50	: .27 -
Limit Test	: no
Analytical monitoring	: no
Method	: other
Year	: 1979
GLP	: yes
Test substance	: other TS
Method	: Used EPA method (1975) 660/3-75-009 Committee on Methods for Toxicity Tests with Aquatic Organisms. Ten <24-h old <i>D. magna</i> Straus were selected from an in-house colony and tested at 20 +/- 1 deg. C in a series of two replicates per test concentration. Test concentrations were 0.056, 0.10, 0.18, 0.32, and 0.56 mg/L, plus clean water and solvent (acetone) controls. Tests were conducted using well water from Columbia, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 25-mL glass beakers containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured for dissolved oxygen, pH, ammonia, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated using EPA statistical procedures.
Remark	: Supplemental information as a previously cited study was used to fulfill HPV requirement.

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Result	: The 24-h EC50 (95% CL) was 0.72 (0.58-0/89) mg/L; the 48-h EC50 (95% CL) was 0.27 (0.21-0.35) mg/L. The NOEC was determined to be 0.056 mg/L. At 24-h, there were no deaths in controls or the lower 4 test concentrations. Clumping of daphnids was observed at the highest three concentrations. At 48-h, there were no deaths in controls or the lowest test concentration, partial deaths in the middle three test levels and 100% deaths in the highest concentration tested. Clumping of daphnids was observed in the highest three concentrations tested. The pH at test initiation was 7.9 and at 48 hrs was 8.3; the DO at 48 hrs was 9.1 mg/L and at test initiation alkalinity and hardness were 368 and 255 mg/l, respectively.	
Test substance	: THERMINOL 88 consisting of 82% Mixed Terphenyls, 16% Quaterphenyls and 2% High Boilers.	
Reliability 19.06.2003	: (2) valid with restrictions	(21)
Type	:	
Species	: Daphnia sp. (Crustacea)	
Exposure period	: 48 hour(s)	
Unit	: mg/l	
LC50	: = .039 -	
Method	: other: calculated (EcoSAR)	
Year	:	
GLP	: no	
Test substance	: other TS	
Remark	: An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR. Data supplied as Supplemental information.	
Test substance 02.06.2003	: Terphenyl [CAS No. 26140-60-3]	(19)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: Selenastrum capricornutum (Algae)	
Endpoint	: other	
Exposure period	: 96 hour(s)	
Unit	: µg/l	
EC50	: 15 -	
EC50 (cell no.)	: 20 -	
Limit test	: no	
Analytical monitoring	: no	
Method	: other	
Year	: 1979	
GLP	: yes	
Test substance	: other TS	
Method	: Used USEPA (1971) Algal Assay Procedure: Bottle Test. National Eutrophication Research Program, Pacific Northwest Water Laboratory, Corvallis, OR. Cultures were incubated at 24 +/- degree C under 4000 lux illumination during a 24-hr photoperiod. Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 3.2, 5.6, 10, 32, and 56 micrograms/L. Both clean water and solvent controls were included. Dimethylformamide (DMF) was used as a cosolvent (0.05 mL/test flask). Test material was dissolved in DMF and directly added to the test vessels. Chlorophyll a was measured using a Turner Model 111 fluorometer. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Specifics of the culture medium were not found. Results were analyzed using probit	

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Result	: analysis and regression analysis. Growth data were analyzed by Student's t-test. PH was maintained between 7.2-7.5 during the test.
Test substance	: Chlorophyl a: 24-h and 48-h EC50 were > 56 microgram/L; 72-h EC50= 29 (95% CI of 3.1-263) microgram/L; 96-h EC50 (95%CI)= 15 (2.8-76) microgram/L. Cell No. 96-h EC50 (95% CL)= 20 (4.7 -86) microgram/L.
Reliability Flag	: (2) valid with restrictions
19.06.2003	: Critical study for SIDS endpoint (22)
Species	: Selenastrum capricornutum (Algae)
Endpoint	: other
Exposure period	: 96 hour(s)
Unit	: µg/l
EC50	: = 103 -
Method	: other
Year	: 1984
GLP	: no data
Test substance	: other TS
Method	: Endpoint evaluated was chlorophyll a, cell number. Cultures were incubated at 22 +/- 1 deg. C. under 4600 lux illumination during a 24-h photoperiod. Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 62.5, 125, 250, 500 and 1000 ug/L. Both clean water and solvent controls were included. Acetone was used as a cosolvent (0.05 mL per test flask). Test material was dissolved in acetone and directly added to the test vessels. Test material was not measured during the test. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Beginning cell counts in the test flasks were 2.0E+4 cells/mL. Specifics of the culture medium were not provided other than stating that test medium was regular algal assay procedure medium. Results were analyzed using USEPA methods (moving average angle method). pH was maintained between 7.0-7.6 during the test.
Remark	: Information provided as Supplemental.
Result	: Cell Number = 96-h EC50 of 103 (95% CI of 86-168) micrograms/L.
Test substance	: Therminol 75 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls and 4% High Boilers.
19.06.2003	(23)
Species	: other algae: green algae
Endpoint	:
Exposure period	: 96 hour(s)
Unit	: mg/l
LC50	: = .031 -
Method	: other: calculated (EcoSAR)
Year	:
GLP	: no
Test substance	: other TS
Remark	: An acute green algal 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR. Information provided as supplemental data in light of available acute aquatic studies cited in this reference.
Test substance	: Terphenyl [CAS No. 26140-60-3]
19.06.2003	(19)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	: Pimephales promelas (Fish, fresh water)
Endpoint	: other
Exposure period	: 34 day(s)
Unit	: mg/l
NOEC	: = .037 -
Analytical monitoring	: yes
Method	: other
Year	: 1986
GLP	: yes
Test substance	: other TS
Method	: Designed to study the early life stage toxicity in Fathead Minnows. < 1 - day old, fertilized embryos were taken from the in-house culture. Flow-through testing was conducted using a modified Brungs proportional diluter over the course of 34 days (including 30 days post hatch). Test solutions were replaced at a rate of 5 times daily. The water supply was local well water which had a range of hardness and alkalinity of 25-36 mg/L and 25-30 mg/L, respectively, as CaCO ₃ . The pH range was 7.0-7.4 and the specific conductance was 100-120 micromhos/cm.
	Fifty embryos were placed into incubation cups, one of which was suspended in each duplicate test 20-L glass aquarium (filled with 15 L) per test concentration and controls. Cups were glass jars with 16-mesh Nitex screen bottoms. Incubation cups were gently oscillated using a rocker arm apparatus. Hatching was deemed complete when no more than 5 unhatched viable embryos remained in any incubation cup (day 4 of exposure). Percent hatch success and survival were recorded.
	Forty live larvae were placed back into their aquaria (from the cups) for 30 days of exposure to assay survival and growth (length and weight). Illumination (16 hr light) was provided by Cool White and Grow Lux fluorescent lights (20-100 foot candles at water surface). Test water was maintained at 25 +/- 1 deg. C. Water quality (temperature, DO, pH, hardness) was measured periodically during the test.
	Five concentrations (mean measured of 0.034, 0.037, 0.064, 0.12, 0.29 mg/L) and an acetone solvent control were used. Test concentrations were measured during the test using GC-FID. Larvae were fed live brine shrimp three times daily and twice daily on weekends. Aquaria were cleaned several times per week. Across all test vessels and throughout the test, DO varied between 7.6 to 8.2 mg/L, temperature was steady at 26 deg. C, hardness varied between 28 and 30 mg/L CaCO ₃ , and pH varied between 6.3-7.5.
Remark	: This study, in conjunction with previously reported acute aquatic studies, provides sufficient information to fulfill the requirements of the HPV program for this endpoint.
Result	: No effects on hatching mortality or success as compared to controls were observed in any test concentration. No effects on larval weight were observed at any test concentration. Survival of larvae and larvae lengths were reduced at 0.064 mg/L, but not at 0.037 mg/L. The overall NOEC for this study was 0.037 mg/L.
Test substance	: Terminol 75 consisted of 62% Terphenyls, 34% Quaterphenyls and 4% High Boilers.
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint

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4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	other	
Value	:	> 5000 - mg/kg bw	
Species	:	rat	
Strain	:	Sprague-Dawley	
Sex	:	male/female	
Number of animals	:	10	
Vehicle	:	other	
Doses	:	5000 mg/kg	
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"	
Year	:	1989	
GLP	:	yes	
Test substance	:	other TS	
Method	:	Limit test conducted using 5M and 5F SD rats 9-12 week old. Test material was suspended in corn oil and dosed at a constant volume of 10 ml/kg by gavage on test day 1. Clinical signs of toxicity were recorded daily, body weights and food consumption were recorded on test day 0, 7 and 14 and all animals necropsied. Temperature, humidity and light cycle were controlled; food and water were given ad libitum.	
Result	:	Preliminary range-find study using 1M and 1F rat per group, resulted in no deaths at dosages of 1,000, 2,000 and 2,600 mg/kg. No deaths occurred in the Limit Test of 5,000 mg/kg. Some reductions in food consumption were noted during the first 4 days after dosing. One female lost weight after 7 days of testing, all other rats at this time point and all rats (including the 1F) gained weight after 14 days. A single animal exhibited urine staining, hypoactivity and unthrifty hair coat during the study. No abnormal observations were noted at necropsy for any animal.	
Test substance	:	Santowax MP consisting of: 99% mixed terphenyls (75% meta, 24 % para, <0.5% ortho-isomer) and 1% quaterphenyls.	
Reliability	:	(1) valid without restriction	
Flag	:	Critical study for SIDS endpoint	
29.04.2003			(25)
Type	:	LD50	
Value	:	= 2604 - mg/kg bw	
Species	:	rat	
Strain	:	Sprague-Dawley	
Sex	:	male/female	
Number of animals	:	50	
Vehicle	:	other	
Doses	:	1,984, 2,500, 3,150, 3,969 and 5,000 mg/kg	
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"	
Year	:	1981	
GLP	:	yes	
Test substance	:	other TS	
Method	:	Groups of 5M and 5F young, adult SD rats were administered one of 5 single doses by gavage of test material in corn oil. Clinical signs of toxicity were recorded each day of the 14-day observation period. All animals were necropsied. Body weights were recorded on study day 0, 7 and 14. Food and water were given ad libitum while temperature, humidity and light cycle were controlled. LD50 determination and 95% CI were calculated by the Probit method of Finny, 1971.	

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Result	: LD50 = 2,604 (95% CI 2247-2940) mg/kg. Occurrence of deaths (in parentheses) at each dose level were: 1,984 mg/kg (1/10), 2,500 mg/kg (6/10), 3,150 mg/kg (6/10), 3,969 mg/kg (10/10), and 5,000 mg/kg (10/10). Deaths occurred within 1-3 days. Sedation, ptosis and ataxia were observed only during the initial day of dosing. Diarrhea, lacrimation, and prostration were seen at later time points. At necropsy, signs were evident of gastrointestinal distress, hemorrhaging and discoloration.
Test substance	: MCS 1980 consisting of 62% Mixed (2% ortho-, 55% meta-, 5% para-)Terphenyls, 34% Quaterphenyls and 4% High Boilers.
Reliability 02.06.2003	: (1) valid without restriction
Type	: LD50
Value	: = 1400 - mg/kg bw
Species	: rat
Strain	: Sprague-Dawley
Sex	: male/female
Number of animals	:
Vehicle	:
Doses	:
Method	: other
Year	: 1962
GLP	: no
Test substance	: other TS
Method	: Groups of 5 rats were administered test material mixed in corn oil by gavage in logarithmically increasing doses between 500-10,000 mg/kg. All survivors were necropsied at study term. LD50 calculated by method of Weil.
Remark	: Provided as supplemental information; results describe the acute oral toxicity of the Mixed Terphenyl material containing a high o-isomer ratio and which was tested in a subsequent Chronic rodent study and reported in section on Repeated Dose.
Result	: LD50 = 1,400 mg/kg
Test substance	: Santowax OM, consisting of 95% Mixed (64% ortho-, 23% meta-, and 6% para-isomers) Terphenyls and < 5% Biphenyl.
Reliability 13.05.2003	: (2) valid with restrictions

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	: Chronic
Species	: rat
Sex	: male/female
Strain	: Long-Evans
Route of admin.	: oral feed
Exposure period	: 235 days
Frequency of treatm.	: daily
Post exposure period	: yes
Doses	: 0.01%, 0.1% and 1.0 %; equivalent to (males/females): 3/3.5 mg/kg/d; 31/37 mg/kg/d; and 350/409 mg/kg/d
Control group	: yes, concurrent vehicle
NOAEL	: = 3.5 - mg/kg bw
Method	: other
Year	: 1965
GLP	: no
Test substance	: other TS
Method	: Groups of 9 male and 9 female rats were administered feed containing either 0.01%, 0.1% or 1.0% test material for up to 235 days. Test material was suspended in corn oil before admix with powdered rat chow. A concurrent vehicle control group was employed. Food and water were provided ad libitum. Animals were housed in wire-mesh caging, 3 rats/cage. Body weights were recorded on day 0 and monthly thereafter; food consumption was also recorded. One third (3 M/3 F) of the rats from each dose group were sacrificed on study days 130, 188 and 235. In an attempt to ascertain reversibility of renal lesions, 3M and 3F fed 1.0% treated diet for 188 days were switched to untreated feed between study days 188 and 235. At final sacrifice, each animal had blood drawn for hematological examination and had its liver, kidneys and lungs weighed, along with a gross necropsy. Histopathologic examination of the following tissues was performed: brain, lungs, heart, stomach, intestines, liver, spleen, pancreas, kidneys, adrenals, urinary bladder, testes, ovaries, and bone. Hematology parameters measured were hemoglobin, hematocrit and white blood cell count. Statistical analysis of mean values for body weight, organ weight and hematology parameters was performed using a t-test. A paired-feeding study, comparing a separate group of 6 rats fed 1.0% treated diet with a feed restricted group of similar size was also performed.
Result	: Mean food test article consumption values for the low, mid and high test group, by sex (M:F) were: 3 and 3.5 mg/kg/d, 31 and 37 mg/kg/d and 350 and 409 mg/kg/d. One female rat fed 1.0% diet died between test days 130-188. No treatment-related effects were observed at 0.01% (3/3.5 mg/kg/d) which is considered the NOEL for this study. At 0.1% (31/37 mg/kg/d) a small reduction in body weight was noted after study day 180 in both males and females. An unidentified pigment was observed in the cytoplasm of some renal tubular cells at this test level. At 1.0% (350/409 mg/kg/d) dramatically lower body weights were observed in both sexes through the first 188 days of testing. Once removed from treated feed, substantive recovery of weight and increased food consumption was observed; final body weights for this group still did not achieve control levels by the end of the study. A statistically significant increase in hemoglobin values was noted at the end of the study for both male and female rats given 1.0% test material in the diet. Rats of both sexes exhibited increased liver weights at the two earlier time points. At the 1.0% test level, rats of both sexes exhibited pathological changes of the kidney consisting of tubular obstruction and an irreversible interstitial nephritis with scarring at both the 130- and 188-day time points. Some signs of partial reversibility of renal lesions was observed in the postdosing study portion. During the paired-feeding study, weight gain was reduced such that this reduction appears test-article related rather than entirely accountable to

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Test substance	: feed palatability.
	: SANTOWAX OM, consisting of 95% Mixed Terphenyls (64% ortho-, 25% meta- and 6% para-) and 5% biphenyl.
Reliability	: (2) valid with restrictions
	: Despite some limitations, these scientifically valid studies assessing prolonged exposure to mixed terphenyls provide sufficient information to complete this HPV endpoint.
Flag	: Critical study for SIDS endpoint
13.05.2003	

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5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Ames test
System of testing	: Salmonella typhimurium strains TA98, TA100, TA1535, and TA1537
Test concentration	: 0.01, 0.04, 0.2, 1.0, 2.0, 3.0, and 10 mg/plate
Cycotoxic concentr.	: equal to or greater than 1 mg/plate
Metabolic activation	: with and without
Result	: positive
Method	: other
Year	: 1982
GLP	: yes
Test substance	: other TS

Method : Method used was plate incorporation assay based on Ames test methods consistent with OECD 471. All tests were run in duplicate and three plates were assayed at each dosage for each run both with and without metabolic activation. The S-9 liver homogenates were prepared from male SD rats and CD-1 mice given Arochlor 1254. All tester strains were obtained from Dr. B. Ames. Sterile DMSO was used as the solvent and a solvent control was employed of 20 uL/plate DMSO. Positive controls used were: 2-aminoanthracene, 9-aminoacridine, benzo(a)pyrene, NaNo₂ and 2-nitrofluorene. A positive response was determined upon observation of a statistically significant dose-response increase in revertant colonies. Bartlett's test was used for pairwise comparison to controls and dose response determined using regression analysis for log-log straight lines; P<0.01 was used.

Result : Positive response with TA100 only with S9; no mutagenic increase with other Salmonella strains with S9 or any strains (including TA100) without S9.

Test substance : MCS 1980 consisting of 62% Mixed Terphenyls and 34% Quaterphenyls and 4% High Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

02.06.2003

(27)

Type	: Cytogenetic assay
System of testing	: Chinese Hamster Ovary Cell In Vitro Assay
Test concentration	: 37.5, 75 and 150 ug/ml
Cycotoxic concentr.	: 150 ug/ml with S9 and 18.8 ug/ml without S9
Metabolic activation	: with and without
Result	: negative
Method	: other
Year	: 1987
GLP	: yes
Test substance	: other TS

Method : Study conducted according to OECD study design, testing involved 2 separate tests with and without S9 fraction added. Fischer male rat Arochlor 1254-induced liver homogenate was used. Cell cultures were handled to prevent photolysis of Brdu-substituted DNA. Each test

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	consisted of concurrent solvent and positive controls and at least 3 dose levels. Cells were incubated in McCoy's 5A medium with test agent ranging between 8-26 hrs, colcemid added to arrest cell division and then harvested/processed. 50 first-division metaphase cells for each dose level in each replication were scored blind from prepared slides for each dose level. Classes of aberrations were recorded and included simple, complex and other abnormalities. Statistical analysis (Chi square pair-wise comparison test) was conducted on individual dose points; significance was determined as $P < 0.05$. A positive response required a statistically significant increase in cells with aberrations or aberrations per cell. Positive controls used (cyclophosphamide and MMS) functioned as expected.	
Remark	: Provided as supplemental information since this chemical has also been tested in an In Vivo Cytogenetics Assay (see subsequent chapter 5.6)	
Result	: No increase in chromosomal aberrations was observed at any dose level at any time point. A top dose level of 150 ug/ml was used as this proved to be the limit of solubility of test material in the solvent (acetone) of choice.	
Test substance	: Santowax R consisting of 81% Mixed Terphenyls and 17% Quarterphenyls and 2% High Boilers.	
Reliability 02.06.2003	: (1) valid without restriction	(28)
Type	: Bacterial reverse mutation assay	
System of testing	: Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, and Saccharomyces yeast D4	
Test concentration	: 0.1, 1.0, 10, 100 and 500 ug/plate	
Cycotoxic concentr.	: 500 ug/plate produced evidence of chemically-induced effect; low dose was without demonstratable toxic effect.	
Metabolic activation	: with and without	
Result	: negative	
Method	: other	
Year	: 1977	
GLP	: no	
Test substance	: other TS	
Method	: Study consistent with OECD 471, using plate overlay method. Duplicate runs conducted, but not run in triplicate. Positive controls used were: MNNG, NF, QM, Anthrace, AAF, and AMQ. Test material dissolved in DMSO. Used S9 fraction obtained from liver of male rats given Arochlor 1254. A response was considered positive in any tester strain, with or without metabolic activation, if 3 concentrations were at least 3X (2X for TA98 and D4) concurrent control values.	
Result	: No mutagenic response observed in any Salmonella tester strains or the D4 Yeast, with or without metabolic activation.	
Test substance	: CP 75052; laboratory synthesized sample of commercial product Therminol 75, consisting of 62% terphenyl, 34% quaterphenyl and 4% High Boilers.	
Reliability 02.06.2003	: (2) valid with restrictions	(29)
Type	: Bacterial reverse mutation assay	
System of testing	: Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, and Saccharomyces yeast D4	
Test concentration	: 0.1, 1.0, 10.0, 100, 500 ug/plate	
Cycotoxic concentr.	: 500 ug/plate produced evidence of chemically-induced effect; low dose was without demonstratable toxic effect.	
Metabolic activation	: with and without	
Result	: negative	
Method	: other	
Year	: 1977	
GLP	: no	
Test substance	: other TS	
Method	: Study consistent with OECD 471, using plate overlay method. Duplicate runs conducted, but not run in triplicate. Positive controls used were:	

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	runs conducted, but not run in triplicate. Positive controls used were: MNNG, NF, QM, Anthrace, AAF, and AMQ. Test material dissolved in DMSO. Used S9 fraction obtained from liver of male rats given Arochlor 1254. A response was considered positive in any tester strain, with or without metabolic activation, if 3 concentrations were at least 3X (2X for TA98 and D4) concurrent control values.	
Result	: No mutagenic response seen in any Salmonella tester strain or D4 yeast, with or without metabolic activation.	
Test substance	: CP 2321 SR (Santowax R) consisting of 81% Mixed Terphenyls and 17% Quaterphenyls and 2% High Boilers.	
Reliability 02.06.2003	: (2) valid with restrictions	(30)
Type	: HGPRT assay	
System of testing	: Chinese Hamster Ovary Cell line	
Test concentration	: 5, 25, 50, 75, and 100 ug/ml	
Cycotoxic concentr.	: 100 ug/ml	
Metabolic activation	: with and without	
Result	: negative	
Method	: OECD Guide-line 476	
Year	: 1984	
GLP	: yes	
Test substance	: other TS	
Method	: CHO cell cultures, prepared from stock cultures originating from Dr. AW Hsie, Oak Ridge National Laboratories, were introduced to flasks containing a density of approximately 5X10E5 cells/flask. After incubation in medium for 16-24 hr cells were removed, washed and 5 ml serum free medium F12, transferred into flasks and test material added directly, diluted in acetone. 1 ml S-9 fractions of male SD rat liver (Arochlor 1254-induced) homogenates (0, 1, 2, 5, and 10%) were added as appropriate. Flasks were gassed with CO2 and incubated for 5 hrs., then medium aspirated, washed and then reincubated an additional 19 hr. Colonies were subcultured in 0.05% trysin solution, cell no. counted and 1000 cells/ml subcultured; 0.2 ml aliquots were plated for survival. Cultures were incubated for up to 7 days and clones fixed, stained and counted for mutant selection. A preliminary cytotoxicity study was run using a range of 7 doses between 0.33 ug/ml-1000 ug/ml and 4 levels of S-9. A Preliminary study using dosages of 20, 50 and 100 ug/ml with and without S9 (0, 1, 2, 5, and 10%) was conducted in duplicate. A Confirmatory test was conducted using final concentrations of 5, 25, 50, 75 and 100 ug/ml with and without 10% S9. Positive controls used were: Ethylmethane sulfonate and Dimethyl nitrosamine. Untreated and solvent-treated controls were also run concurrently. This test was run in triplicate. Statistical treatment of raw data was performed using a computer program obtained from J.Irr (EPA) to evaluate mutation frequency. One way ANOVA was used on transformed mutation frequency data according to methodology supplied by Snee and Irr (1981). p<0.01.	
Remark	: Supplementary information regarding the lack of genotoxicity observed in a mammalian cell line point mutation as say.	
Result	: Cytotoxicity was complete at 333 ug/ml and significant at 100 ug/ml. No statistically significant differences in mutation frequency between treated and control doses were observed with or without any of the S9 fractions used. A dose-dependent trend was noted in cells treated with 10% S9 in the Preliminary Study. In the Confirmatory Study, no statistically significant increases in mutation frequency or trend were observed either with or without 10% S9. Positive and negative controls performed as expected.	
Test substance	: MCS 1980 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls and 4% High Boilers.	
Reliability 23.07.2003	: (2) valid with restrictions	(31)

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Type	:	HGPRT assay
System of testing	:	Chinese Hamster Ovaries cells
Test concentration	:	10, 50, 100, 250, & 500 ug/ml (without S9); 1, 5, 10, 25, 50, 75, and 100 ug/ml (with S9)
Cycotoxic concentr.	:	16.7 ug/ml and higher
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476
Year	:	1986
GLP	:	yes
Test substance	:	other TS
Method	:	<p>CHO cell cultures, prepared from stock cultures originating from Dr. AW Hsie, Oak Ridge National Laboratories, were introduced to flasks containing a density of approximately 5X10E5 cells/flask. After incubation in medium for 16-24 hr cells were removed, washed and 5 ml serum free medium F12, transferred into flasks and test material added directly, diluted in acetone. 1 ml S-9 fractions of male SD rat liver (Arochlor 1254-induced) homogenates (0, 1, 2, 5, and 10% S9) were added as appropriate. Flasks were gassed with CO2 and incubated for 5 hrs., then medium aspirated, washed and then reincubated an additional 19 hr. Colonies were subcultured in 0.05% trysin solution, cell no. counted and 1000 cells/ml subcultured; 0.2 ml aliquots were plated for survival. Cultures were incubated for up to 7 days and clones fixed, stained and counted for mutant selection. A preliminary cytotoxicity study was run using a range of 8 doses between 0.167 ug/ml-500 ug/ml and 4 levels of S-9. A Preliminary study, using dosages of 5, 10 and 25 ug/ml with 1% & 2% S9 as well as 5, 50, 100 and 500 (without S9) ug/ml each with and without 5 and 10% S9, was conducted in duplicate. A Confirmatory test was conducted using final concentrations of 5, 25, 50, 75 and 100 ug/ml with 5% S9 and 1, 5, 10, 25, 50, 75, and 100 ug/ml in the absence of S9. Positive controls used were: Ethylmethane sulfonate and Dimethyl nitrosamine. Untreated and solvent-treated controls were also run concurrently. This test was run in triplicate. Due to unfavorable response in the positive control, this experiment was conducted three times before minimum acceptable standards were met. Statistical treatment of raw data was performed using a computer program obtained from J.Irr (EPA) to evaluate mutation frequency. One way ANOVA was used on transformed mutation frequency data according to methodology supplied by Snee and Irr (1981). p<0.01.</p>
Remark	:	Supplementary information regarding the lack of genotoxicity observed in a mammalian cell line point mutation assay.
Result	:	Cytotoxicity was seen at 16.7 ug/ml and limits of solubility exceeded at test levels of 167 and 500 ug/ml; deminished cytotoxicity appeared at doses for 50 and 100 ug/ml in the presence of S9. No statistically significant differences in mutation frequency between treated and control doses were observed with or without any of the S9 fractions used. Similarly, in the Confirmatory Study, no statistically significant increases in mutation frequency or trend were observed either with our without 1-10% S9. Positive and negative controls performed as expected in the definitive Confirmatory study.
Test substance	:	Santowax R
Reliability	:	(2) valid with restrictions
27.05.2003		

(32)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344

Route of admin.	:	i.p.
Exposure period	:	once with sampling periods of 6, 12 and 24 hrs.
Doses	:	500, 2500, and 5,000 mg/kg body weight
Result	:	negative
Method	:	OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone Marrow Cytogenetic Test - Chromosomal Analysis"
Year	:	1985
GLP	:	yes
Test substance	:	other TS
Method	:	Dose levels selected based on pilot study were no effects were seen up to 5000 mg/kg test agent, the highest dose used in this study design. Six Fischer-344 rats/sex/time period were administered test agent in corn oil by intraperitoneal injection. Metaphase cells were collected from rat bone marrow (femur) at harvest times of 6, 12 and 24 hrs after treatment. Colchicine was administered 2 hr prior to sacrifice to arrest cells in c-metaphase. Marrow was exposed to hypotonic solution and fixed, cells and slides prepared and stained. All slides were coded before reading. Positive and negative (corn oil and untreated) controls were used for comparative purposes. Mitotic index was calculated based on counting of at least 1000 slides and chromosomal aberrations evaluated from at least 60 slides per animal per time point from the untreated control groups (male and female) and the 5,000 mg/kg test groups. All breaks, deletions, translocations and other changes were recorded. Mitotic Index, % chromosomally aberrant cells and frequency of chromosomal aberrations per cell were compared between treated vs control groups using ANOVA and Dunnett's test. P <0.05 was used.
Result	:	No toxicologically significant effects were noted at any dose level, nor where there any deaths observed during the study. No increase in mitotic index, % aberrant cells or aberrations per cell were noted in either male or female rats evaluated after 6, 12, or 24 hrs following treatment at 5000 mg/kg test material.
Test substance	:	Therminol 75 consisting of 62% Mixed Terphenyls and 34% Quaterphenyls and 4% High Boilers.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint
02.06.2003		

(33)

5.7 CARCINOGENICITY**5.8.1 TOXICITY TO FERTILITY****5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY****5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES**

Type	:	other
In vitro/in vivo	:	In vivo
Species	:	rat
Sex	:	male/female
Strain	:	Long-Evans
Route of admin.	:	oral feed
Exposure period	:	235 days
Frequency of treatm.	:	daily
Duration of test	:	

5. Toxicity

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Doses	:	0.01, 0.1 and 1.0 % (approx. 3/3.5, 31/37 and 350/409 mg/kg/d for males and females, respectively)
Control group	:	yes, concurrent vehicle
Result	:	No histopathological effects noted on testes or ovaries after 130, 188 or 235 days of testing.
Method	:	other
Year	:	1965
GLP	:	no
Test substance	:	other TS
Remark	:	This information has been summarized extensively in the Repeated Dose Toxicity section of this monograph. While this data is insufficient for purposes of completely addressing this HPV endpoint, it does provide useful information indicative of a lack of histopathologic findings which could affect reproductive performance.
Test substance	:	Santowax OM consisting of 95% Mixed Terphenyls (64% ortho-, 25% meta- and 6% para-) and 5% biphenyl.
Reliability 29.04.2003	:	(2) valid with restrictions

(26)

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

- (1) Monsanto technical report bulletin 7239531, 1999.
- (2) Monsanto Co. Technology study. Cite on Solutia MSDS. 1980
- (3) MPBPWIN. Version 1.40. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (4) Monsanto Technical report and cited on Solutia MSDS, 1990.
- (5) Monsanto technical report, ES-83-SS-66
- (6) Neely, W.B. and G.E. Blau. 1985. Environmental Exposure from Chemicals. CRC Press. IN Syracuse Research Corporation (SRC). Physical Properties (PhysProp) Database. <http://esc.syrres.com/interkow/PhysProp.htm> (accessed September 18, 2002).
- (7) Sangster, J. (Sangster Research Laboratories, Montreal, Canada). 1993. Octanol-Water Partition Coefficients: Fundamentals and Physical Chemistry. Wiley, New York. 178p. IN Syracuse Research Corporation (SRC). Physical Properties Database (PhysProp). <http://esc.syrres.com/intekow/PhysProp.htm> (accessed September 18, 2002).
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- (9) Meylan, W.M. and P.H. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. Journal of Pharmaceutical Sciences. 84(1): 83-92. IN Syracuse Research Corporation (SRC). Physical Properties (PhysProp) Database. <http://esc.syrres.com/interkow/PhysProp.htm> (accessed September 18, 2002).
- (10) Solutia Study No. MO-02-0445. Aqueous Solubility of MCS 1980.
- (11) Solutia internal PRM memo, 12/28/79 summarizing findings.
- (12) Meylan, WM, PH Howard and RS Boethling. 1996. Improved method for estimating water solubility from octanol/water partition coefficient. Environ. Toxicol and Chem 15(2): 100-106. IN Syracuse Research Corp. Physical Properties (PhysProp) Database.
- (13) AOPWIN. Version 1.90. Atmospheric Oxidation. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (14) Solutia Study No. MO20020694. Biodegradation Testing of THERMINOL 55 and THERMINOL 88.
- (15) Solutia Study no. MO-02-385. Biodegradation Screen of MCS-1980.
- (16) Solutia Study no. XX-88-9289. Fate Testing For Therminol Biodegradation.
- (17) Solutia Study no. XX-84-X107; Acute Toxicity of Therminol 75 to Fathead Minnows.
- (18) Solutia Study no. AB-79-318B. Acute Toxicity of Therminol 88 to Rainbow Trout.
- (19) USEPA EcoSAR model (v. 0.99f).
- (20) Solutia Study No. MO-84-X044; Acute Toxicity of MCS 1980 New to Daphnia magna.
- (21) Solutia Study No. AB-79 -317. Acute Toxicity of THERMINOL 88 to Daphnia magna.
- (22) Solutia Study No. BN-79-316. Toxicity of THERMINOL 88 to Freshwater Alga Selenastrum capricornutum.

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- (23) Solutia Study No. XX-84-X080; Toxicity of Therminol 75 to the Freshwater Green Alga *Selenastrum capricornutum*.
 - (24) Solutia Study No. SB-98-59; The Toxicity of Therminol 75 to Fathead Minnow Embryos and Larvae.
 - (25) Solutia Study No. BD-88-406; Acute Oral Toxicity in Rats: SANTOWAX MP.
 - (26) Petkau, A and J Hoogstraaten. 1965. Chronic Toxicity of Polyphenyl Mixtures. *Amer. Indust. Hyg. Assoc. J.* 26: 380-387 and also in: Young, G, A Petkau, and J Hoogstraten. 1969. Chronic Toxic Effects of Polyphenyl Mixtures. *Amer. Ind. Hyg. Assoc. J.* 30: 7-19.
 - (27) Solutia Study No. DA-82-240. Salmonella Mutagenicity Assay of MCS-1980.
 - (28) Solutia Study No. SR-86-413; 1986a. An Assessment of Clastogenic Potential of SANTOWAX R Utilizing the Mammalian Cytogenic Assay with CHO Cells
 - (29) Solutia Study No. BO-77-327; Mutagenicity Evaluation of CP 75052.
 - (30) Solutia Study No. BO-77-328. Mutagenicity evaluation of CP 2321 SR.
 - (31) Solutia Study no. PK-84-149. 1984. CHO/HGPRT Mammalian Cell Forward Gene Mutation Assay: THERMINOL 75.
 - (32) Solutia Study no. PK-86-411. 1986. CHO/HGPRT Mammalian Cell Forward Gene Mutation Assay: SANTOWAX R.
 - (33) Solutia Study No. SR-84-414; An Assessment of the Mutagenic Potential of THERMINOL 75 Utilizing the Acute In Vivo Rat Bone Marrow Cytogenetics Assay.

10. Summary and Evaluation

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 92-06-8
CASNo. : 92-06-8
Common name : meta-terphenyl
TSCA Name : m-terphenyl
EINECS Name : m-terphenyl
EC No. : 202-122-1
Molecular Formula : C18H14

Producer related part

Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part

Company : Solutia Inc.
Creation date : 17.03.2003

Status :
Memo :

Printing date : 23.07.2003
Revision date :
Date of last update : 09.07.2003

Number of pages : 23

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1. General Information

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1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 87 - °C
Sublimation :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
19.06.2003 (1) (2)

2.2 BOILING POINT

Value : = 363 - °C at
Decomposition :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
19.06.2003 (1) (2)

2.3 DENSITY**2.3.1 GRANULOMETRY****2.4 VAPOUR PRESSURE**

Value : = .0000233 - hPa at 25 °C
Decomposition :
Method : other (measured): not reported
Year :
GLP : no data
Test substance : other TS

Remark : Reported as 1.75×10^{-5} mm Hg @ 25 deg. C.
Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Daubert and Danner. 1992
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
19.06.2003 (3)

2. Physico-Chemical Data

Id 92-06-8
Date 23.07.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 5.52 - at °C
pH value : -
Method : other (calculated): atom/fragment contribution method
Year :
GLP : no
Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for 130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and correction factors for a given chemical structure.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Meylan and Howard. 1995
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
09.07.2003 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = 1.51 - mg/l at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : slightly soluble (0.1-100 mg/L)
Stable :
Deg. product :
Method : other: measured, method not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Yalkowsky and Dannenfelser. 1992.
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
19.06.2003 (5)

Solubility in : Water
Value : .11 - at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year : 1984
GLP : no

2. Physico-Chemical Data

Id 92-06-8
Date 23.07.2003

Test substance	:	other TS
Method	:	Estimation of aqueous solubility was based on plotting the aqueous solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: $\log(RT) = -0.1946 \log(uS) + 1.091$ with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS=aqueous solubility in u moles/L. A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient development.
Remark	:	Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Result	:	Estimation of the aqueous solubility using the Calibration Curve method was 0.11 ppm while estimation of correlation with the Kow derived an estimate of 0.67 ppm.
Test substance	:	m-Terphenyl
Reliability	:	(2) valid with restrictions
19.06.2003		

(6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : water
 Light source : Sun light
 Light spectrum : - nm
 Relative intensity : - based on intensity of sunlight

DIRECT PHOTOLYSIS

Half-life t_{1/2} : = 140 - day(s)
 Degradation : 14 - % after 29 day(s)
 Quantum yield :
 Deg. product :
 Method : other (measured)
 Year : 1983
 GLP : no
 Test substance : other TS

Method : A 20 ppm solution of m-terphenyl was prepared in a 50:50 mixture of deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp. reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame ionization detector. Triplicate extracts were analyzed at 20 ppm and a single extraction at 2 ppm.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : A half-life of 140 day was calculated. Approximately a 14% decrease in concentration was observed after 29 days of sunlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight:dark control were : day 0 (100%), day 1 (105/108%), day 3 (98/96%), day 7 (86/96%), day 14 (103/113%) and day 29 (76/88%). The absorbance of a 20 ppm acetonitrile:water (50:50) solution of m-Terphenyl at 290 nm was 0.24/cm pathlength.

Test substance : Meta-Terphenyl from Monsanto Chemicals procurement lab; purity unspecified.

Reliability : (2) valid with restrictions
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(7)

Type : other
 Light source :
 Light spectrum : - nm
 Relative intensity : - based on intensity of sunlight
 Deg. product :
 Method : other (calculated): AOPWIN v1.90
 Year :
 GLP : no
 Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
 Vapor phase m-terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction

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with hydroxyl radicals was calculated as $12.66E-12 \text{ cm}^3/(\text{molecule} \cdot \text{sec})$.
Based on $1.5E6 \text{ OH molecules/cm}^3$ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 20.3 hours.

Source : EPIWIN
Test substance : m-Terphenyl [CAS No. 92-06-8]
Reliability : (2) valid with restrictions
19.06.2003 (8)

3.1.2 STABILITY IN WATER

Remark : The test substance (m-Terphenyl) is not susceptible to hydrolysis.
13.05.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air-water-soil-sediment
Air : .87 % (Fugacity Model Level I)
Water : 11.8 % (Fugacity Model Level I)
Soil : 45 % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : 42.4 % (Fugacity Model Level II/III)
Method : other
Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). Physical properties of m-terphenyl used as the model input parameters were: water solubility = 1.51 mg/L, vapor pressure = $1.75E-5 \text{ Hg}$; log Kow = 5.52; melting point = 87 deg. C. All property values were taken from this Robust Summary.

Remark : Air: half life = 20.3 hr; emissions = 1000 kg/hr
Water: half life = 900 hr; emissions = 1000 kg/hr
Soil: half life = 900 hr, emissions = 1000 kg/hr
Sediment: half life = 3600 hr; emissions = 1000 kg/hr

Persistence Time: 972 hr
Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Test substance : m-Terphenyl
Reliability : (2) valid with restrictions
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3.3.2 DISTRIBUTION

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3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other
Concentration : 20 mg/l related to Test substance
related to
Contact time : 55 day(s)
Degradation : 38 - (\pm) % after 55 day(s)
Result :
Deg. product :
Method : other
Year : 1983
GLP : no
Test substance : other TS

Method : Ultimate biodegradation screening study using a shake flask carbon dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3×10^8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg $(\text{NH}_4)_2 \text{SO}_4$ per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO_2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to verify methodology.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : Following 55 days of exposure, a mean (3 reps) level of 38% (SD = 18) with range of 19-53% CO_2 evolution was achieved.

Test substance : Sample of m-Terphenyl obtained from Monsanto Co. Chemical Procurement Laboratory with confirmed GC purity of >95%.

Reliability : (2) valid with restrictions
19.06.2003

(9)

Type : aerobic
Inoculum : other: Mississippi River Water
Contact time :
Degradation : 100 - (\pm) % after 28 day(s)
Result : other: Biodegradable after long acclimation period
Deg. product :
Method : other: River Die Away Test
Year : 1983
GLP : no
Test substance : other TS

Method : Samples of Mississippi River water (suspended solids= 51 mg/L; pH = 8.25; microbial colonies/ml = 5.5×10^4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were

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and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whereby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.

- Remark** : Supplemental information which supports the conclusion that m-Terphenyl is capable of biological degradation in the environment.
- Result** : After a relatively long (16-day) acclimation period, m-Terphenyl rapidly degraded (complete degradation by test day 28) during both the first and second trial.
- Test substance** : meta-Terphenyl, obtained from the Monsanto Procurement Laboratory, with GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers used in the Mixture trial also were verified as > 95% pure.
- Reliability** : (2) valid with restrictions

19.06.2003

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3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	other: fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .084 -
Method	:	other: calculated (EcoSAR)
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.
Remark	:	Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Test substance	:	m-Terphenyl [CAS No. 92-06-8]
13.05.2003		

(11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	>= .011 -
EC50	:	= .022 -
Analytical monitoring	:	no
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	other TS
Method	:	Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at an ave. temp. of 21.2 deg. C in a series of three replicates per test concentration. Test concentrations were 0.011, 0.018, 0.03, 0.05 and 0.083 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to preclude volatilization and used well water from St. Peters, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 8 oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated using EPA statistical procedures.
Remark	:	Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Result	:	48-h EC50 (95% CL) = 0.022 mg/L (0.019-0.025 mg/L). NOEC = 0.011 mg/L. % immobility (in parenthesis) seen after 24-h: control (0), solvent control (3), 0.011 mg/L (0), 0.018 mg/L (10), 0.03 mg/L (13), 0.05 mg/L (7), and 0.083 mg/L (37); and at 48-hr: control (0), solvent control (3), 0.011 mg/L (7), 0.018 mg/L (37), 0.03 mg/L (73), 0.05 mg/L (93), and 0.083 mg/L (100). pH ranged from 7.8-8.2; DO ranged from 6.0-8.3; alkalinity ranged from 186-204 mg/L CaCO ₃ ; hardness ranged from 180-198 mg/L CaCO ₃ .

4. Ecotoxicity

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Test substance : Analytical grade sample of m-Terphenyl; purity unknown.
Reliability : (2) valid with restrictions
19.06.2003 (12)

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = .115 -
Method : other: calculated (EcoSAR)
Year :
GLP : no
Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.
Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Test substance : m-Terphenyl [CAS No. 92-06-8]
13.05.2003 (11)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green algae
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .088 -
Method : other: calculated (EcoSAR)
Year :
GLP : no
Test substance : other TS

Method : An acute green algal 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Test substance : m-Terphenyl [CAS No. 92-06-8]
13.05.2003 (11)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4. Ecotoxicity

Id 92-06-8
Date 23.07.2003

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type : LD50
Value : = 2400 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals :
Vehicle : other
Doses : 500-10,000 mg/kg
Method : other (calculated)
Year : 1962
GLP : no
Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its codification. Groups of 5 male and female SD rats were administered test material in logarithmically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. LD50 and CI were calculated according to the method of Weil. After determination of the LD50 additional groups of 5 rats were administered the test article in a similar fashion at dosages of 1000, 2000 and 4000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and observation of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necropsies were performed and histopathological examinations were conducted on the following organs: heart, liver, lung, adrenals, kidneys and spleen.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]. Study adequate to provide corroborative information in assessment of Mixed Terphenyls.

Result : LD50=2,400 mg/kg (95% CL=1600-3700). At 1000 mg/kg, no deaths occurred and only a short-term (1-2 day) weight loss was observed. Similar signs seen at 2000 mg/kg, although 2 deaths were reported. At 4000 mg/kg acute distress was observed within 3-5 hrs followed by vocalization upon touch; deaths occurred within 48 hrs. No histopathological effects were reported for any test group and liver and kidney weight ratios relative to body weight were considered normal.

Test substance : Reagent grade meta-terphenyl, verified for purity but unspecified.

Reliability : (2) valid with restrictions

19.06.2003

(13)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES**

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	: Sub-acute
Species	: rat
Sex	: no data
Strain	: Sprague-Dawley
Route of admin.	: oral feed
Exposure period	: 30 days
Frequency of treatm.	: daily
Post exposure period	: none
Doses	: 500, 250 and 100 mg/kg body weight
Control group	: yes
NOAEL	: = 100 - mg/kg bw
Method	: other
Year	: 1962
GLP	: no
Test substance	: other TS
Method	: Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was available ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all test levels
Result	: 100 mg/kg - Overall NOEL. At 250 mg/kg/d - Slight reduction in body weight at the end of the study; Liver weight and ratio were statistically elevated; no discernable effects on kidney wt. or histopathology of any organ. At 500 mg/kg/d - A significant reduction in body weight was observed at the end of the study. Liver weight /ratio were statistically elevated but Kidney weight/ratio were normal. No histopathological effects noted in organs examined.
Test substance	: Reagent grade meta -terphenyl purchased from Eastman Chemical and confirmed for purity.
Reliability	: (2) valid with restrictions Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers found in Mixed Terphenyls.

13.05.2003

(13)

Type	: Sub-acute
Species	: rat
Sex	: male
Strain	: Wistar
Route of admin.	: oral feed
Exposure period	: 14 days
Frequency of treatm.	: daily
Post exposure period	: none
Doses	: 0.2 % in the diet (2000 ppm)
Control group	: yes
LOAEL	: = .2 - %

5. Toxicity

Id 92-06-8

Date 23.07.2003

Method : other
Year : 1974
GLP : no
Test substance : other TS

Method : An unspecified number of young, adult male Wistar rats were administered commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necropsy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and liver cholesterol. Unspecified statistical methods used with $p < 0.05$.

Result : After 14 days of testing, a significant (8%) reduction in body weight was observed, along with a statistical increase (136%) in plasma cholesterol level, but not liver cholesterol. Food consumption was reduced statistically as were adrenal, kidney, liver and spleen weights. Liver hypertrophy was reported.

Test substance : Meta-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.
Reliability : (4) not assignable
Provided as Supplemental information.

13.05.2003 (14)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Salmonella typhimurium reverse mutation assay
System of testing : TM 677
Test concentration : several concentrations up to the limit of solubility of 900 μM
Cycotoxic concentr. :
Metabolic activation : with
Result : negative
Method : other
Year : 1979
GLP : no
Test substance : other TS

Method : Salmonella exposed to test material concentrations for 2 hr in the presence of 10% postmitochondrial supernatant (obtained separately from phenobarbital and Arochlor pretreated male SD rats) along with cofactors supporting metabolic activation. Bacteria were centrifuged, resuspended and plated under selective and nonselective conditions. Mutant colonies were counted after 48 hr growth at 37 deg. F and the ratio of mutations on selective vs nonselective media examined. Positive response was considered on basis of achieving a mutation fraction higher than the 99%CL of the mean background fraction.

Result : When tested up to the maximum level of solubility using both phenobarbital and Arochlor S9 fractions, no evidence of mutagenic response was observed.

Test substance : Sample of meta-Terphenyl obtained from Annalabs, Inc. North Haven, Conn. Purity unspecified.

Reliability : (4) not assignable
Supplementary information provided on one isomeric component of Mixed Terphenyls.

22.04.2003 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type	:	other
In vitro/in vivo	:	In vitro
Species	:	mouse
Sex	:	male/female
Strain	:	other
Route of admin.	:	other
Exposure period	:	20-24 hr incubation
Frequency of treatm.	:	once
Duration of test	:	
Doses	:	0, 0.1, 1, 10 ug/mL.
Control group	:	other
Result	:	Statistical decrease in IVF & increased abnormal embryos and degenerative oocytes at 1 and 10 ug/mL.
Method	:	other
Year	:	1994
GLP	:	no
Test substance	:	other TS
Method	:	Used the mouse in vitro fertilization (IVF) technique to measure effects on fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test concentration. Mean scores were statistically evaluated using Chi Square and Bonferroni Chi Square Contingency Tables with p<0.05.
Remark	:	Supplemental information; study inadequate to support this HPV endpoint.
Result	:	No treatment-related effects were observed at 0.1 ug/mL A statistically significant decrease in FIV and increases in abnormal embryos and degenerative oocytes were observed at 1 and 10 ug/mL
Test substance	:	Purchased from AccuStandard, Inc. CT and verified by GC -FID as 99% pure m-terphenyl.
Reliability	:	(3) invalid
19.06.2003		

(16)

5. Toxicity

Id 92-06-8
Date 23.07.2003

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 92-06-8
Date 23.07.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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- (2) Syracuse Research Corporation (SRC). Physical Properties (PhysProp) Database. <http://esc.syrres.com/interkow/PhysProp.htm> (accessed September 18, 2002).
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- (9) Solutia Study no. MO20020705; Ultimate biodegradation screening of selected polyphenyls and hydrogenated polyphenyls.
- (10) Solutia Study no. MO20020457. River Die Away Testing of Some Polyphenyls and Some Partially Hydrogenated Polyphenyls.
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- (12) Solutia Study no. MO1983X076; Acute toxicity of m-Terphenyl to Daphnia magna.
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10. Summary and Evaluation

Id 92-06-8
Date 23.07.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 84-15-1
CASNo. : 84-15-1
TSCA Name : ortho-Terphenyl

Producer related part
Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part
Company : Solutia Inc.
Creation date : 17.03.2003

Status :
Memo :

Printing date : 23.07.2003
Revision date :
Date of last update : 23.07.2003

Number of pages : 25

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1. General Information

Id 84-15-1
Date 23.07.2003

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 56.2 - °C
Sublimation :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
19.06.2003 (1) (2)

2.2 BOILING POINT

Value : = 332 - °C at
Decomposition :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
19.06.2003 (1) (2)

2.3 DENSITY**2.3.1 GRANULOMETRY****2.4 VAPOUR PRESSURE**

Value : = .0003 - hPa at 25 °C
Decomposition :
Method : other (measured): not reported
Year :
GLP : no data
Test substance : other TS

Remark : Reported as 0.00025 mm Hg @ 25 deg. C.
Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Daubert and Danner. 1989
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
19.06.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 5.28 - at °C
pH value : -
Method : other (measured): not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Source : Ogata et al. 1984
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
 19.06.2003 (4)

Partition coefficient : octanol-water
Log pow : = 5.52 - at °C
pH value : -
Method : other (calculated): atom/fragment contribution method
Year :
GLP : no
Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for 130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and correction factors for a given chemical structure.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Source : Meylan and Howard. 199
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
 19.06.2003 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in Value : Water
 : = 1.24 - mg/l at 25 °C
pH value concentration : -
 : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : slightly soluble (0.1-100 mg/L)
Stable :
Deg. product :
Method : other: measured, method not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Source : Yalkowsky and Dannenfelser. 1992
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

2. Physico-Chemical Data

Id 84-15-1
Date 23.07.2003

19.06.2003

(6)

Solubility in : Water
Value : .83- at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year : 1983
GLP : no
Test substance : other TS

Method : Estimation of aqueous solubility was based on plotting the aqueous solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: $\log(RT) = -0.1946 \log(uS) + 1.091$ with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS=aqueous solubility in u moles/L.

A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient development.

Remark : Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : Estimation of the aqueous solubility using the Calibration Curve method was 0.83 ppm while estimation of correlation with the Kow derived an estimate of 5.5 ppm.

Test substance : o-Terphenyl

Reliability : (2) valid with restrictions

19.06.2003

(7)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2. Physico-Chemical Data

Id 84-15-1
Date 23.07.2003

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 84-15-1
Date 23.07.2003

3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight

DIRECT PHOTOLYSIS

Half-life t_{1/2} : -
Degradation : < 8 - % after 29 day(s)
Quantum yield :
Deg. product :
Method : other (measured)
Year : 1983
GLP : no
Test substance : other TS

Method : A 20 ppm solution of o-terphenyl was prepared in a 50:50 mixture of deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp. reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame ionization detector. Triplicate extracts were analyzed at 20 ppm and a single extraction at 2 ppm.

Remark : Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : No significant decrease in concentration was observed after 29 days of sunlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight/dark control were: day 0 (100%), day 1 (86/96%), day 3 (93/95%), day 7 (95/89%), day 14 (95/98%) and day 29 (92/91%). The absorbance of a 20 ppm acetonitrile:water (50:50) solution of o-Terphenyl at 290 nm was 0.13/cm pathlength.

Test substance : Ortho-Terphenyl from Monsanto Chemicals procurement lab; purity unspecified.

Reliability : (2) valid with restrictions

19.06.2003

(8)

Type : other
Light source :
Light spectrum : - nm
Relative intensity : - based on intensity of sunlight
Deg. product :
Method : other (calculated): AOPWIN v1.90
Year :
GLP : no
Test substance : other TS

Remark : Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Vapor phase o-terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as $9.1946E-12 \text{ cm}^3/(\text{molecule} \cdot \text{sec})$. Based on $1.5E6 \text{ OH molecules/cm}^3$ and assuming 12 hours of sunlight per
8 / 25

3. Environmental Fate and Pathways

Id 84-15-1
Date 23.07.2003

Based on 1.5E6 OH molecules/cm³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 27.9 hours.

Source : EPIWIN
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions
19.06.2003 (9)

3.1.2 STABILITY IN WATER

Remark : Test substance (o-Terphenyl) is not susceptible to hydrolysis.
13.05.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air-water-soil-sediment
Air : 1.29 % (Fugacity Model Level I)
Water : 14.7 % (Fugacity Model Level I)
Soil : 50.9 % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : 33 % (Fugacity Model Level II/III)
Method : other
Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). Physical properties of o-terphenyl used as the model input parameters were water solubility of 1.24 mg/L; vapor pressure of 0.00025 mm Hg; log Kow of 5.28, and melting point of 56.2 deg. C. All property values were taken from this Robust Summary.

Remark : Air: half life = 27.9 hr; emissions = 1000 kg/hr
Water: half life = 900 hr; emissions = 1000 kg/hr
Soil: half life = 900 hr; emissions = 1000 kg/hr
Sediment: half life = 3600 hr; emissions = 0 kg/hr

Persistence Time: 853 hr.
Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Reliability : (2) valid with restrictions
09.07.2003

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3. Environmental Fate and Pathways

Id 84-15-1

Date 23.07.2003

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other
Concentration : related to Test substance
related to
Contact time : 55 day(s)
Degradation : = 20 - (\pm 34) % after 55 day(s)
Result :
Deg. product :
Method : other
Year : 1983
GLP : no
Test substance : other TS

Method : Ultimate biodegradation screening study using a shake flask carbon dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3×10^8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH₄)₂ SO₄ per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO₂ level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to verify methodology.

Remark : Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : Following 55 days of exposure, a mean (3 reps) level of 20% (SD = 34) with range of 0 -60% CO₂ evolution was achieved.

Test substance : Sample of o-Terphenyl obtained from Monsanto Chemical Procurement Laboratory with confirmed GC purity of > 95%.

Reliability : (2) valid with restrictions
23.07.2003

(10)

Type : aerobic
Inoculum : other: Mississippi River Water
Contact time :
Degradation : 100 - (\pm) % after 42 day(s)
Result : other: Biodegradable after long acclimation period
Deg. product :
Method : other: River Die Away test
Year : 1983
GLP : no
Test substance : other TS

Method : Samples of Mississippi River water (suspended solids= 51 mg/L; pH = 8.25; microbial colonies/ml = 5.5×10^4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28.

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sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whereby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.

Remark : Supplemental information which supports the conclusion that o-Terphenyl is capable of biological degradation in the environment.

Result : After a long (28-day) acclimation period, o-Terphenyl rapidly degraded (complete degradation by test day 42) during the second trial.

Test substance : ortho-Terphenyl, obtained from the Monsanto Procurement Laboratory, with GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers used in the Mixture trial also were verified as > 95% pure.

Reliability : (2) valid with restrictions

23.07.2003 (11)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	other: fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .084 -
Method	:	other: calculated (EcoSAR)
Year	:	
GLP	:	no
Test substance	:	other TS
Remark	:	An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR. Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Test substance	:	o-Terphenyl [CAS No. 84-15-1]
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4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	>= .036 -
EC50	:	= .045 -
Analytical monitoring	:	no
Method	:	other
Year	:	1983
GLP	:	yes
Test substance	:	other TS
Method	:	Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at 20 +/- 1 deg. C in a series of three replicates per test concentration. Test concentrations were 0.022, 0.036, 0.06, 0.1 and 0.167 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to preclude volatilization and used well water from St. Peters, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 8-oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated using EPA statistical procedures.
Remark	:	Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Result	:	48-h EC50 (95% CL) = 0.045 mg/L (0.036-0.060 mg/L). NOEC = 0.036 mg/L. % immobility (in parenthesis) seen after 24-h: control (0), solvent control (0), 0.022 mg/L (0), 0.036 mg/L (0), 0.06 mg/L (13), 0.1 mg/L (27), and 0.167 mg/L (60); and at 48-hr: control (0), solvent control (3), 0.022 mg/L (0), 0.036 mg/L (0), 0.06 mg/L (13), 0.1 mg/L (27), and 0.167 mg/L (60). pH ranged from 7.8-8.3; DO ranged from 7.5-8.4; alkalinity ranged from 186-206 mg/L CaCO3; hardness ranged from 180-194 mg/L CaCO3.

4. Ecotoxicity

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Test substance : Analytical grade sample o-Terphenyl; purity unknown.
Reliability : (2) valid with restrictions
13.05.2003 (13)

Type :
Species : Daphnia sp. (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : = .115 -
Method : other: calculated (EcoSAR)
Year :
GLP : no
Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.
Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Test substance : o-Terphenyl [CAS No. 84-15-1]
13.05.2003 (12)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green algae
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .088 -
Method : other: calculated (EcoSAR)
Year :
GLP : no
Test substance : other TS

Remark : An acute green algal 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.
Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Test substance : o-Terphenyl [CAS No. 84-15-1]
09.07.2003 (12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4. Ecotoxicity

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4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type : LD50
Value : = 1900 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals :
Vehicle : other
Doses : 500-10,000 mg/kg
Method : other (calculated)
Year : 1962
GLP : no
Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its codification. Groups of 5 male and female SD rats were administered test material in logarithmically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. LD50 and CI were calculated according to the method of Weil. After determination of the LD50 additional groups of 5 rats were administered the test article in a similar fashion at dosages of 500, 1000 and 2000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and observation of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necropsies were performed and histopathological examinations were conducted on the following organs: heart, liver, lung, adrenals, kidneys and spleen.

Remark : Study adequate to provide corroborative information in assessment of mixed terphenyls. Provided as Supplemental information.

Result : LD50=1,900 mg/kg (1300-2800 mg/kg). Generalized signs of toxicity were observed in most animals, including rough coat and diarrhea. At 2000 and 1000 mg/kg: Two deaths occurred at 2000 mg/kg within 4 days and 1 death at 1000 mg/kg during the same period; animals exhibited cataplectic behavior and vocalization when touched within 8 days of dosing. The liver- and kidney-to-body weight ratios were normal at all dose levels. No effects were observed at 500 mg/kg.

Test substance : Reagent grade ortho-terphenyl, with purity verified but unspecified.

Reliability : (2) valid with restrictions

19.06.2003

(14)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES**

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	: Sub-acute
Species	: rat
Sex	: no data
Strain	: Sprague-Dawley
Route of admin.	: oral feed
Exposure period	: 30 days
Frequency of treatm.	: daily
Post exposure period	: none
Doses	: 500, 250 and 100 mg/kg/d body weight
Control group	: yes
NOAEL	: = 100 - mg/kg bw
Method	: other
Year	: 1962
GLP	: no
Test substance	: other TS
Method	: Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was available ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all test levels
Result	: 100 mg/kg - Overall NOEL. AT 250 mg/kg/d - Slight reduction in body weight at the end of the study; Liver weight/ratio and kidney weight/ratio were statistically elevated; no discernable effects on histopathology of any organ. At 500 mg/kg/d - A significant reduction in body weight with rats losing 10-15 gm from their initial group weight after the first 10 days of testing. After 30 days on test, lost weight had been regained but 30-day value was substantially below control value. The Liver weight /ratio and Kidney weight/ratio were statistically elevated at study's end. No histopathological effects noted in organs examined.
Test substance	: Reagent grade ortho-terphenyl purchased from Eastman Chemical and confirmed for purity but unspecified.
Reliability	: (2) valid with restrictions Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers found in Mixed Terphenyls.

29.04.2003

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Type	: Sub-acute
Species	: rat
Sex	: male
Strain	: Wistar
Route of admin.	: oral feed
Exposure period	: 14 days
Frequency of treatm.	: daily
Post exposure period	: none
Doses	: 0.2% in the diet (2000 ppm)

5. Toxicity

Id 84-15-1

Date 23.07.2003

Control group : yes
LOAEL : = .2 - %
Method : other
Year : 1974
GLP : no
Test substance : other TS

Method : An unspecified number of young, adult male Wistar rats were administered commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necropsy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and liver cholesterol. Unspecified statistical methods used with $p < 0.05$.

Result : After 14 days of testing, a significant (15%) reduction in body weight was observed, along with an increased plasma cholesterol level (121%). Food consumption was reduced statistically as were adrenal and kidney weights. Adrenal hypertrophy was reported.

Test substance : Ortho-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.
Reliability : (4) not assignable
Provided as Supplemental information.

13.05.2003

(15)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Salmonella typhimurium reverse mutation assay
System of testing : TM677
Test concentration : several concentrations up to the limit of solubility of 900 μ M
Cycotoxic concentr. :
Metabolic activation : with
Result : negative
Method : other
Year : 1979
GLP : no
Test substance : other TS

Method : Salmonella exposed to test material concentrations for 2 hr in the presence of 10% postmitochondrial supernatant (obtained separately from phenobarbital and Arochlor pretreated male SD rats) along with cofactors supporting metabolic activation. Bacteria were centrifuged, resuspended and plated under selective and nonselective conditions. Mutant colonies were counted after 48 hr growth at 37 deg. F and the ratio of mutations on selective vs nonselective media examined. Positive response was considered on basis of achieving a mutation fraction higher than the 99%CL of the mean background fraction.

Result : When tested up to the maximum level of solubility using both phenobarbital and Arochlor S9 fractions, no evidence of mutagenic response was observed.

Test substance : Sample of ortho-Terphenyl obtained from Annalabs, Inc. North Haven, Conn. Purity unspecified.

Reliability : (4) not assignable
Supplementary information provided on one isomeric component of Mixed Terphenyls.

22.04.2003

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5.6 GENETIC TOXICITY 'IN VIVO'

5. Toxicity

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5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other
In vitro/in vivo : In vitro
Species : mouse
Sex : male/female
Strain : other
Route of admin. : other
Exposure period : 20-24 hr incubation
Frequency of treatm. : once
Duration of test :
Doses : 0, 0.1, 1, 10 ug/mL.
Control group : yes
Result : Increased number of abnormal embryos and degenerative oocytes at and above 1 ug/mL.
Method : other
Year : 1994
GLP : no
Test substance : other TS

Method : Used the mouse in vitro fertilization (IVF) technique to measure effects on fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test concentration. Mean scores were statistically evaluated using Chi Square and Bonferroni Chi Square Contingency Tables with $p < 0.05$.

Remark : Supplemental information; study inadequate to support this HPV endpoint.
Result : Statistically decreased IVF and increased number of abnormal embryos and degenerative oocytes at and above 1 ug/mL
Test substance : Purchased from AccuStandard, Inc. CT and verified by GC -FID as 99% pure ortho-Terphenyl
Reliability : (3) invalid

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5. Toxicity

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5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10. Summary and Evaluation

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 92-94-4
CASNo. : 92-94-4
Common name : para-terphenyl
TSCA Name : p-Terphenyl
EINECS Name : p-terphenyl
EC No. : 202-205-2

Producer related part
Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part
Company : Solutia Inc.
Creation date : 17.03.2003

Status :
Memo :

Printing date : 23.07.2003
Revision date :
Date of last update : 23.07.2003

Number of pages : 24

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1. General Information

Id 92-94-4
Date 23.07.2003

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value : = 210.1 - °C
Sublimation :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : SRC PhysProp Database.
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions
19.06.2003 (1)

2.2 BOILING POINT

Value : = 376 - °C at
Decomposition :
Method : other: not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database.
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions
19.06.2003 (2) (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .000000456 - hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Remark : Reported as 3.42×10^{-7} mm Hg @ 25 deg. C.
Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Neely and Blau. 1985.
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions
19.06.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 6.03 - at °C
pH value : -
Method : other (measured): not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Sangster. 1993
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions
 19.06.2003

(4)

Partition coefficient : octanol-water
Log pow : = 5.52 - at °C
pH value : -
Method : other (calculated): atom/fragment contribution method
Year :
GLP : no
Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for 130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and correction factors for a given chemical structure.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Meylan and Howard. 1995.
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions
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(5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .0018 - mg/l at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : insoluble (< 0.1 mg/L)
Stable :
Deg. product :
Method : other: measured, method not reported
Year :
GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Source : Yalkowsky and Dannenfelser. 1992
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions

2. Physico-Chemical Data

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(6)

Solubility in : Water
Value : .055 - at 25 °C
pH value : -
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other
Year : 1983
GLP : no
Test substance : other TS

Method : Estimation of aqueous solubility was based on plotting the aqueous solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: $\log(RT) = -0.1946 \log(uS) + 1.091$ with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS=aqueous solubility in u moles/L.

A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient development.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : Estimation of the aqueous solubility using the Calibration Curve method was 0.055 ppm while estimation of correlation with the Kow derived an estimate of 0.023 ppm.

Test substance : p-Terphenyl

Reliability : (2) valid with restrictions

19.06.2003

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2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2. Physico-Chemical Data

Id 92-94-4
Date 23.07.2003

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water	
Light source	:	Sun light	
Light spectrum	:	- nm	
Relative intensity	:	- based on intensity of sunlight	
Deg. product	:		
Method	:	other (measured)	
Year	:	1983	
GLP	:	no	
Test substance	:	other TS	
Method	:	A 10 ppm solution of p-terphenyl was prepared in a 50:50 mixture of deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp. reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame ionization detector. Triplicate extracts were analyzed at 10 ppm and a single extraction at 2 ppm.	
Remark	:	Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]	
Result	:	No significant decrease (<10%) in concentration was observed after 29 days of sunlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight/dark control were within experimental error. They were: day 0 (100%), day 1 (62/93%), day 3 (107/111%), day 7 (93/97%), day 14 (108/115%) and day 29 (90/101%). The absorbance of a 10 ppm acetonitrile:water (50:50) solution of p-Terphenyl at 290 nm was 1.18/cm pathlength.	
Test substance	:	Para-Terphenyl from Aldrich Chemical;purity unspecified.	
Reliability 19.06.2003	:	(2) valid with restrictions	
			(8)
Type	:	other	
Light source	:		
Light spectrum	:	- nm	
Relative intensity	:	- based on intensity of sunlight	
Deg. product	:		
Method	:	other (calculated): AOPWIN v1.90	
Year	:		
GLP	:	no	
Test substance	:	other TS	
Remark	:	Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3] Vapor phase p-terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 9.1946E-12 cm ³ /(molecule*sec). Based on 1.5E6 OH molecules/cm ³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 27.9 hours.	
Test substance	:	p-Terphenyl [CAS No. 92-94-4]	
Reliability	:	(2) valid with restrictions	

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(9)

3.1.2 STABILITY IN WATER

Remark : The test substance (p-Terphenyl) is not susceptible to hydrolysis.
13.05.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media : other: air-water-soil-sediment
Air : 1.06 % (Fugacity Model Level I)
Water : 11.7 % (Fugacity Model Level I)
Soil : 45.3 % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : 41.9 % (Fugacity Model Level II/III)
Method : other
Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). The following physical properties of p-terphenyl were used as model input parameters: water solubility = 0.0018 mg/L; vapor pressure of 3.42E-7 mm Hg; log Kow = 5.52; melting point = 210.1 deg. C. All property values were from this Robust Summary.

Remark : Air: half life = 27.9 hr; emissions = 1000 kg/hr
Water: half life = 900 hr; emissions = 1000 kg/hr
Soil: half life = 900 hr; emissions = 1000 kg/hr
Sediment: half life = 3600 hr; emissions = 0 kg/hr

Conclusion : Persistence Time: 986 hr
: Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Reliability : (2) valid with restrictions
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3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic

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Inoculum	: domestic sewage
Concentration	: 20 mg/l related to Test substance 10 mg/l related to Test substance
Contact time	: 42 day(s)
Degradation	: 0 - (\pm) % after 42 day(s)
Result	: under test conditions no biodegradation observed
Deg. product	:
Method	: other: 42-day shake flask ultimate biodegradation
Year	: 1991
GLP	: yes
Test substance	: other TS
Method	: Two test concentrations, 10 and 20 mg/L nominal, standard BOD medium enhanced with 2 times normal amount of phosphate buffer, 4 times normal amount of FeCL ₃ , and 40 mg (NH ₄) ₂ SO ₄ per liter purified water; two liter triplicate flasks fitted with barium hydroxide solutions to catch CO ₂ , sodium benzoate positive control. HgCL ₂ -treated sterile control, inocula from acclimated solution prepared using 8-week SCAS procedure: activated mixed liquor plus raw filtered sewage, 1500 mL in glass vessels, stirred, aerated, suspended solids of 2500 to 5000 mg/L, 24-h cycle at end of which it was settled for 30 min, 1L decanted, 1L raw sewage added containing test substance at 1 mg/cycle via acetone. Initial bacterial count in test vessels inoculated with SCAS preparation was 6.1E+5 CFU/mL. At final day, residue analyzed using RP-HPLC-UV for remaining test material. Test vessels were incubated at 27 +/- 2 deg. C. in the dark on a rotary shaker.
Remark	: Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]
Result	: For the positive control, ~ 100 % thCO ₂ formed; for nominal 10 mg/L test substance, 9% thCO ₂ formed; for 20 mg/L test material, 8% thCO ₂ formed. Analysis of day 42 residue showed that 81% and 78% remained, respectively, in tests using 10 and 20 mg/L test material. For the sterile control, 82% remained. NO volatile losses were reported. It was concluded that no appreciable degradation had occurred with the test substance.
Test substance	: p-Terphenyl made up of 97.9% para, 1.7% meta- and 0.3% ortho-Terphenyl isomer.
Reliability	: (1) valid without restriction
13.05.2003	(10)
Type	: aerobic
Inoculum	: other
Concentration	: 20 mg/l related to Test substance related to
Contact time	: 55 day(s)
Degradation	: = 10 - (\pm 14) % after 55 day(s)
Result	:
Deg. product	:
Method	: other
Year	: 1983
GLP	: no
Test substance	: other TS
Method	: Ultimate biodegradation screening study using a shake flask carbon dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10 ⁸ colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH ₄) ₂ SO ₄ per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was

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	<p>supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO₂ level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to verify methodology.</p>	
Remark	: Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]	
Result	: Following 55 days of exposure, a mean (3 reps) level of 10% (SD = 14) with range of 0 -26% CO ₂ evolution was achieved.	
Test substance	: Sample of p-Terphenyl obtained from Aldrich, with confirmed GC purity of >95%.	
Reliability 09.07.2003	: (2) valid with restrictions	(11)
Type	: aerobic	
Inoculum	: other:Mississippi River water	
Contact time	:	
Degradation	: 0 - (±) % after 42 day(s)	
Result	: under test conditions no biodegradation observed	
Deg. product	:	
Method	: other: River Die Away Test	
Year	: 1983	
GLP	: no	
Test substance	: other TS	
Method	: Samples of Mississippi River water (suspended solids= 51 mg/L; pH = 8.25; micorbial colonies/ml = 5.5x10E4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whereby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.	
Remark	: Supplemental information which supports the conclusion that p-Terphenyl is resistant to biological degradation in the environment.	
Result	: Even after a long (42-day) acclimation period, no appreciable biodegradation occurred with p-Terphenyl in either Trial.	
Test substance	: para-Terphenyl, obtained from the Monsanto Procurement Laboratory, with GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers used in the Mixture trial also were verified as > 95% pure.	
Reliability 03.06.2003	: (2) valid with restrictions	(12)

3.6 BOD₅, COD OR BOD₅/COD RATIO

3.7 BIOACCUMULATION

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3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type :
Species : other: fish
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = .028 -
Method : other: calculated (EcoSAR)
Year :
GLP : no
Test substance : other TS

Remark : An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.

Test substance : p-Terphenyl [CAS No. 92-94-4]
Conclusion : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

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4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
NOEC : > 5.5 -
EC50 : > 5.5 -
Analytical monitoring : no
Method : other
Year : 1983
GLP : yes
Test substance : other TS

Method : Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at 20 +/- 1 deg. C in a series of three replicates per test concentration. Test concentrations were 0.344, 0.688, 1.375, 2.75 and 5.5 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to preclude volatilization and used well water from St. Peters, Mo. Photoperiod employed was unspecified. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 8-oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]

Result : 48-h EC50 > 5.5 mg/L. NOEC > 5.5 mg/L. % immobility (in parenthesis) seen after 24-h: control (0), solvent control (0), 0.344 mg/L (0), 0.688 mg/L (0), 1.375 mg/L (0), 2.75 mg/L (0), and 5.5 mg/L (3); and at 48-hr: control (0), solvent control (0), 0.344 mg/L (0), 0.688 mg/L (0), 1.375 mg/L (0), 2.75 mg/L (3), and 5.5 mg/L (3). pH ranged from 7.8-8.0; DO ranged from 8.0-8.7; alkalinity ranged from 256-262 mg/L CaCO₃; hardness ranged from 230-244 mg/L CaCO₃. Visual inspection of all test containers indicated that the water solubility level of this chemical was exceeded. In a range-find study, at nominal test concentrations (0.005, 0.01, 0.05, and 0.1

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range-find study, at nominal test concentrations (0.005, 0.01, 0.05, and 0.1 mg/L) below visual indications of insolubility, no more than 1 % immobility was observed.

Test substance	: Analytical grade sample p-Terphenyl; purity unknown.	
Reliability	: (2) valid with restrictions	(14)
23.07.2003		
Type	:	
Species	: Daphnia sp. (Crustacea)	
Exposure period	: 48 hour(s)	
Unit	: mg/l	
LC50	: = .039 -	
Method	: other: calculated (EcoSAR)	
Year	:	
GLP	: no	
Test substance	: other TS	
Remark	: An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.	
Test substance	: p-Terphenyl [CAS No. 92-94-4]	
Conclusion	: Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]	
13.05.2003		(13)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: other algae: green algae	
Endpoint	:	
Exposure period	: 96 hour(s)	
Unit	: mg/l	
LC50	: = .031 -	
Method	: other: calculated (EcoSAR)	
Year	:	
GLP	: no	
Test substance	: other TS	
Remark	: An acute green algal 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.	
Test substance	: p-Terphenyl [CAS No. 92-94-4]	
Conclusion	: Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]	
13.05.2003		(13)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

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4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type : LD0
Value : > 10000 - mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals :
Vehicle : other
Doses : 500-10000 mg/kg
Method : other (calculated)
Year : 1962
GLP : no
Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its codification. Groups of 5 male and female SD rats were administered test material in logarithmically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. After determination of the LD0 additional groups of 5 rats were administered the test article in a similar fashion at dosages of 2000, 4000 and 10000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and observation of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necropsies were performed and histopathological examinations were conducted on the following organs: heart, liver, lung, adrenals, kidneys and spleen.

Remark : Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3]. Study adequate to provide corroborative information in assessment of mixed terphenyls.

Result : LD0 > 10,000 mg/kg Consistent signs of toxicity were observed in most animals, including rough coat and diarrhea. However, no deaths occurred at 10,000 mg/kg (highest dose tested). No effects noted in body weights or necropsy or histopathology, with the exception of possible liver regeneration.

Test substance : Reagent grade para-terphenyl, with purity verified but unspecified.

Reliability : (2) valid with restrictions

13.05.2003

(15)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES****5.2.1 SKIN IRRITATION**

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type : Sub-acute
Species : rat
Sex : no data
Strain : Sprague-Dawley
Route of admin. : oral feed
Exposure period : 30 days
Frequency of treatm. : daily
Post exposure period : none
Doses : 500, 250 and 100 mg/kg body weight
Control group : yes
NOAEL : = 250 - mg/kg bw
Method : other
Year : 1962
GLP : no
Test substance : other TS

Method : Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was administered ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all test levels

Result : 250 mg/kg - Overall NOEL. At 500 mg/kg/d - A significant reduction in body weight was observed at the end of the study. No treatment-related effects were noted in liver or kidney weights/weight ratios or after histopathological examination of organs.

Test substance : Reagent grade para-terphenyl purchased from Eastman Chemical and confirmed for purity but unspecified.

Reliability : (2) valid with restrictions
 Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers found in Mixed Terphenyls.

29.04.2003

(15)

Type : Sub-acute
Species : rat
Sex : male
Strain : Wistar
Route of admin. : oral feed
Exposure period : 14 days
Frequency of treatm. : daily
Post exposure period : none
Doses : 0.2 % in the diet (2000 ppm)
Control group : yes
LOAEL : = .2 - %
Method : other
Year : 1974
GLP : no
Test substance : other TS

5. Toxicity

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Method : An unspecified number of young, adult male Wistar rats were administered commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necropsy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and liver cholesterol. Unspecified statistical methods used with $p < 0.05$.

Result : After 14 days of testing a significant increase (118%) in plasma cholesterol level was observed. No other effects noted at this test level.

Test substance : Para-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.

Reliability : (4) not assignable
Provided as Supplemental information.

13.05.2003

(16)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other
In vitro/in vivo : In vitro
Species : mouse
Sex : male/female
Strain : other
Route of admin. : other
Exposure period : 20-24 hr incubation
Frequency of treatm. : once
Duration of test :
Doses : 0, 0.1, 1, and 10 ug/mL
Control group : yes
Result : Increased number of abnormal embryos and degenerative oocytes at and above 1 ug/mL.

Method : other
Year : 1994
GLP : no data
Test substance : other TS

Method : Used the mouse in vitro fertilization (IVF) technique to measure effects on fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controlled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to

motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test concentration. Mean scores were statistically evaluated using Chi Square and Bonferroni Chi Square Contingency Tables with $p < 0.05$.

- Remark** : Supplemental information; study inadequate to support this HPV endpoint.
Result : No treatment-related effects were observed at 0.1 ug/mL. An increase in the number of embryos and degenerative oocytes was observed at 1 and 10 ug/mL. No overall statistically significant decrease in IVF was reported although there was a small decrease in IVF at 10 ug/mL vs control.
- Test substance** : Purchased from AccuStandard, Inc. CT and verified by GC-FID as 99% pure para-Terphenyl
- Reliability** : (3) invalid
19.06.2003

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5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical : ID: 29036-02-0
CAS No. : 29036-02-0
Common name : Quaterphenyl
EINECS Name : Quaterphenyl
Molecular Formula : C₂₄H₁₈
EC No. : 249-380-1

Producer related part
Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part
Company : Solutia Inc.
Creation date : 17.03.2003

Status :
Memo :

Printing date : 23.07.2003
Revision date :
Date of last update : 23.07.2003

Number of pages : 20

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1. General Information

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1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	160 - 200 °C	
Sublimation	:		
Method	:	other: Internal analysis	
Year	:	1990	
GLP	:		
Test substance	:	other TS	
Test substance	:	Santotar 9 consisting of a 100% polyphenyl mixture made up of 95% Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.	
Reliability	:	(2) valid with restrictions	
Flag	:	Critical study for SIDS endpoint	
09.07.2003			(1)
Value	:	= 184.1 °C	
Sublimation	:		
Method	:	other: calculated (MPBPWIN v1.40)	
Year	:		
GLP	:	no	
Test substance	:	other TS	
Source	:	EPIWIN	
Test substance	:	Quaterphenyl [CAS No. 29036-02-0]	
Reliability	:	(2) valid with restrictions	
09.07.2003			(2)

2.2 BOILING POINT

Value	:	> 420 °C at	
Decomposition	:		
Method	:	other: Internal analysis	
Year	:	1990	
GLP	:		
Test substance	:	other TS	
Test substance	:	Santotar 9 consisting of a 100% polyphenyl mixture made up of 95% Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.	
Reliability	:	(2) valid with restrictions	
Flag	:	Critical study for SIDS endpoint	
23.07.2003			(3)
Value	:	= 481.2 °C at	
Decomposition	:		
Method	:	other: calculated (MPBPWIN v1.40)	
Year	:		
GLP	:	no	
Test substance	:	other TS	
Source	:	EPIWIN	
Test substance	:	Quaterphenyl [CAS No. 29036-02-0]	
Reliability	:	(2) valid with restrictions	
09.07.2003			(2)

2.3 DENSITY

2. Physico-Chemical Data

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2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00000000237 hPa at 25 °C
Decomposition :
Method : other (calculated): MPBPWIN v1.40
Year :
GLP : no
Test substance : other TS

Remark : Reported as 1.78e-9 mm Hg @ 25 deg. C.
Source : EPIWIN
Test substance : Quaterphenyl [CAS No. 29036-02-0]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
09.07.2003 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = 7.28 at °C
pH value :
Method : other (calculated): KOWWIN v1.66
Year :
GLP : no
Test substance : other TS

Source : EPIWIN
Test substance : Quaterphenyl [CAS No. 29036-02-0]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
19.06.2003 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : .002 at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: Internal analysis
Year : 1990
GLP : yes
Test substance : other TS

Method : Used two water samples (tap and well water) and analyzed via LC methodology with confirmed detection limit to 0.000102 mg/L.
Test substance : Santotar 9 consisting of a 100% polyphenyl mixture made up of 95% Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.

2. Physico-Chemical Data

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Reliability	:	(1) valid without restriction	
Flag	:	Critical study for SIDS endpoint	
09.07.2003			(5)
Solubility in Value	:	Water	
pH value concentration	:	= .00677 mg/l at 25 °C	
Temperature effects	:		
Examine different pol.	:		
pKa	:	at 25 °C	
Description	:	insoluble (< 0.1 mg/L)	
Stable	:		
Deg. product	:		
Method	:	other: calculated (WSKOW v1.37)	
Year	:		
GLP	:	no	
Test substance	:	other TS	
Source	:	EPIWIN	
Test substance	:	Quaterphenyl [CAS No. 29036-02-0]	
Reliability	:	(2) valid with restrictions	
09.07.2003			(6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : other
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
Deg. product :
Method : other (calculated): AOPWIN v1.90
Year : 2002
GLP : no
Test substance : other TS

Remark : Vapor phase quaterphenyls are susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as $18.544E-12$ cm³/(molecule*sec). Based on $1.5E6$ OH molecules/cm³ and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 13.8 hours.

Source : EPIWIN
Test substance : Quaterphenyl [CAS No. 29036-02-0]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
23.07.2003

(7)

3.1.2 STABILITY IN WATER

Remark : The test substance (Quaterphenyl) is not susceptible to hydrolysis. It has only 4-membered aromatic rings associated with its structure, which are listed in Lyman in Table 7.1- Types of Organic Functional Groups That Are Generally Resistant to Hydrolysis. Lyman, WJ, Reehl, WF and Rosenblatt, DH. 1990. Handbook of Chemical Property Estimation Methods. Environmental Behaviour of Organic Compounds. American Chemical Society, Washington, DC.

02.06.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : .218 % (Fugacity Model Level I)
Water : 3.47 % (Fugacity Model Level I)
Soil : 32.3 % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : 64.1 % (Fugacity Model Level II/III)

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Method : other
Year : 2002

Method : Used EPIWIN (2002), Syracuse Research Corp, Syracuse, NY. Physical properties of quaterphenyl used as the model input parameters were water solubility of 0.00677 mg/L, vapor pressure of 1.78E-9 mm Hg, log Kow of 7.28, and melting point point of 184.1 deg. C. All property values were taken from this IUCLID dossier.

Remark : Air: half-life = 13.8 hr, emissions = 1000 kg/hr
Water: half-life = 900 hr; emissions = 1000 kr/hr
Soil: half-life = 900 hr, emissions= 1000 kg/hr.
Sediment: half-life = 3600 hr, emissions = 0 kg/hr

Persistence Time - 1740

Test substance : Quaterphenyls [CAS no. 29036-02-0]
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
23.07.2003

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : other
Concentration : 20 mg/l related to Test substance
related to

Contact time : 55 day(s)
Degradation : = 7 (±9) % after 55 day(s)
Result :
Deg. product :
Method : other
Year : 1983
GLP : no
Test substance : other TS

Method : Ultimate biodegradation screening study using a shake flask carbon dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10E8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH4)2 SO4 per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to verify methodology.

3. Environmental Fate and Pathways

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verify methodology.
Result : Following 55 days of exposure, a mean (3 reps) level of 7% (SD=9) with a range of 0-16% CO2 evolution was achieved.
Test substance : Sample of Quaterphenyl isomer with a verified (GC) purity of > 95% and obtained from the Monsanto Chemical Procurement Laboratory.
Reliability Flag : (2) valid with restrictions
 Critical study for SIDS endpoint
 23.07.2003 (8)

Type : aerobic
Inoculum :
Contact time :
Degradation : 54 (±) % after 7.5 month
Result :
Deg. product :
Method : other: Soil microbial biodegradation
Year : 1988
GLP : no
Test substance : other TS

Method : Used a defined methodology to determine the degree of biodegradability caused by soil microorganisms from two separate soil samples. Two concentrations of test material (50 ppm and 0.5 ppm) were prepared in methylene chloride. Two soil types, (1) Missouri Bottoms, a sandy soil with 0.5% organic carbon and a moisture content of 11.3% at 1/3 BAR and (2) Florida muck, a heavy loam containing 32.9% organic carbon and an 82% moisture content at 1/3 BAR. Soil samples containing test material were analyzed by HPLC after 0, 0.5, 1, 2, 4, 6, 8, 12, 15, and 32 weeks on study. A microtox screen was employed prior to study start to insure no bacterial toxicity would interfere with the subsequent test. Method of detection of test material was validated on both soils pres tudy. Soil samples were stabilized prior to study start such that they contained a uniform level of microorganisms. Soil samples (25 gm) were placed in 125 ml jars and spiked with 250 ul of test solution containing the test material in solvent. Jars were capped and shaken, then lids removed and restirred manually. After being lightly recapped, the jars containing the test material and soil were incubated in the dark at 25 deg. C and 80% humidity until sampled. Three replicates of each treated group plus a control per time period per soil type were used. Sterile controls and matrix blanks were also employed. Kinetic parameters were calculated from raw data.

Remark : Provided as Supplementary information.
Result : % Reduction Relative to Nominal Concentration after 32 Weeks on Test

Nominal Conc.	% Red.	Soil Type	% Vs Sterile Soil	T 1/2 (weeeks)
500 ppm	54	Mo. Bott.	-35	28.9
0.5 ppm	50	Mo. Bott.	-	32.0
500 ppm	42	Fla Muck	27	40.9
0.5 ppm	33	Fla Muck	-	54.7

Quaterphenyl underwent little biological degradation upon introduction to either sandy or loam soil types containing soil bacteria. The degree of loss seen in the sandy soil was essentially the same as seen in the sterilized control. Thus, most of the loss observed in nonsterile soil was considered abiotic. Some biologically-mediated degradation was observed in the Fla. Muck soil.

Test substance : Sample labeled "Quaterphenyls"
Reliability : (2) valid with restrictions
 19.06.2003 (9)

3. Environmental Fate and Pathways

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3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	other: fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .002
Method	:	other: calculated (EcoSAR)
Year	:	
GLP	:	no
Test substance	:	other TS
Remark	:	An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.
Test substance	:	Quaterphenyl [CAS No. 29036-02-0]
13.05.2003		(10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	flow through
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
NOEC	:	= .008
EC50	:	>= .069
Analytical monitoring	:	yes
Method	:	other: EPA 660/3-75-009, 560/6-82-002
Year	:	1993
GLP	:	yes
Test substance	:	other TS
Method	:	Ten <24-h old D. magna Straus were tested at 20 +/- 1 deg C. in a series of two replicates per test concentration. Nominal test concentrations were 0.006, 0.012, 0.025, 0.05, and 0.1 mg/L, plus clean water and solvent (dimethylformamide) control. A half-liter proportional diluter system was used to introduce TS. One liter glass beakers with notched drains covered with 50-mesh stainless steel screen were used as the test chamber. Tests were conducted using reconstituted water prepared to a total hardness of 130 to 160 mg/L CaCO3. Concentrations were measured analytically. Daphnids were not fed during the test. Lighting was on a 16-h day: 8-h night cycle with 30 min. transition periods. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test.
Result	:	Water quality was measured for dissolved oxygen, pH and temperature and no significant changes were observed in any parameter during the test. Statistical analyses were performed according to USEPA procedures. Mean measured concentrations of the TS were 0.004, 0.008, 0.016, 0.031 and 0.069 mg/L. Daphnids were observed to surface at the 0.016 mg/L level and above. All solutions were considered visually clear. Temperature ranged from 20-21 deg.C, pH ranged from 8.2-8.4, DO ranged from 7.4 to 8.0 mg/L, hardness ranged from 134 to 146 mg/L as CaCO3, alkalinity was 160 mg/L CaCO3. Immobilizations ranged between 0 and 10% across all concentrations and controls at both the 24-h and 48-h time points. 24-h EC50 = > 0.069 mg/L 48-h EC50 = > 0.069 mg/L

	48-h EC50 = > 0.069 mg/L NOEC = 0.008 mg/L.	
Test substance	: Santotar 9, a 100% polyphenyl mixture made up of 95% Quaterphenyls and 5% Mixed Terphenyls.	
Reliability Flag	: (1) valid without restriction	
19.06.2003	: Critical study for SIDS endpoint	(11)
Type	:	
Species	: Daphnia sp. (Crustacea)	
Exposure period	: 48 hour(s)	
Unit	: mg/l	
LC50	: = .004	
Method	: other: calculated (EcoSAR)	
Year	:	
GLP	: no	
Test substance	: other TS	
Remark	: An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.	
Test substance	: Quaterphenyl [CAS No. 29036-02-0]	
Reliability	: (2) valid with restrictions	
15.05.2003		(10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	: other algae: green algae	
Endpoint	:	
Exposure period	: 96 hour(s)	
Unit	: mg/l	
LC50	: = .003	
Method	: other: calculated (EcoSAR)	
Year	:	
GLP	: no	
Test substance	: other TS	
Remark	: An acute green algal 96-h LC50 was calculated using ECOSAR, from the USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR.	
Test substance	: Quaterphenyl [CAS No. 29036-02-0]	
13.05.2003		(10)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA**4.5.1 CHRONIC TOXICITY TO FISH****4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES****4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS**

4. Ecotoxicity

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4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION**5.1.1 ACUTE ORAL TOXICITY**

Type	:	LD50
Value	:	= 5650 - mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other
Doses	:	3980, 5010, 6310, and 7940 mg/kg
Method	:	other (calculated)
Year	:	1974
GLP	:	no
Test substance	:	other TS
Method	:	Groups of 5 mixed sex young adult rats were administered logarithmically spaced dosages of test material by single gavage dose. Each dosage was prepared as a 20% suspension in corn oil, after heating to 115 Deg. F. Observations for toxicity were made daily for 14 consecutive days. All animals underwent a necropsy. Food and water were provided ad libitum; humidity, temperature and light cycle were controlled. Body weights were recorded on test days 0, 7 and 14. LD50 value and CI were determined by the method of Litchfield and Wilcoxon, 1949.
Remark	:	Study conducted according to OECD 401 design but with some limitations (i.e., smaller sample size); however, results are sufficiently robust to support this endpoint for HPV program.
Result	:	LD50 (95% CL) = 5,650 (5370-5930) mg/kg. Most deaths occurred within 4 days. No. dead/5 animals (in parenthesis) per test group: 1980 mg/kg (0/5), 5010 mg/kg (1/5), 6310 mg/kg (4/5), and 7940 mg/kg (5/5). Generalized signs of toxicity (data not available for individual animals) included weakness, reduced appetite and hypoactivity. Liver discoloration and acute gi inflammation were observed in decedents at necropsy; viscera of all survivors appeared normal at necropsy.
Test substance	:	Santowax Q, consisting of 95% Quaterphenyls and 5% Mixed Terphenyls.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
23.07.2003		

(12)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES****5.2.1 SKIN IRRITATION****5.2.2 EYE IRRITATION**

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

- (1) Monsanto Internal technical report, cited on Solutia MSDS, 4/3/02.
- (2) MPBPWIN. Version 1.40. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (3) Monsanto Internal Technical report, cited on Solutia MSDS, 4/3/02.
- (4) KOWWIN. Version 1.66. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (5) Solutia study no. MO-90-9561. 1990. Determination of Santotar 9 in water.
- (6) WSKOW. Version 1.37. EPIWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (7) AOPWIN. Version 1.90. Atmospheric Oxidation. EPWIN (Estimation Program Interface for Windows). Version 3.05. Syracuse Research Corporation. Syracuse, NY. (EPIWIN, 2000)
- (8) Solutia Study no. MO20020705. 1983. Ultimate biodegradation screening of selected polyphenyls and hydrogenated polyphenyls.
- (9) Solutia Study no. XX-88-9289. Fate Testing For Therminol Biodegradation.
- (10) USEPA EcoSAR model (v. 0.99f).
- (11) Solutia Study no. AB-93-9118. 1993. Acute Flow-Through Toxicity of Santotar 9 to Daphnia magna.
- (12) Solutia Study no. Y-73-273. 1974. Toxicological Investigation of Santowax Q.

10. Summary and Evaluation

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT