REACH

Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Bu and pentyl) esters, zinc salts

EC number: 273-527-9 | CAS number: 68988-45-4

Ecotoxicological information

Short-term toxicity to aquatic invertebrates

Administrative data

Endpoint:	short-term toxicity to aquatic invertebrates
Type of information:	experimental study
Adequacy of study:	key study
Study period:	1993 - 1994
Reliability:	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies:	other: Study conducted in compliance with agreed protocols, without deviations from standard test guidelines. Analytical measurements on test material not conducted except for TOC

Data source

Reference

Reference Type:	study report
Title:	Unnamed
Year:	1994
Report date:	1994

Materials and methods

Test guideline

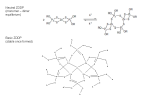
Qualifier:	according to guideline
Guideline:	OECD Guideline 202 (Daphnia sp. Acute Immobilisation Test)
Deviations:	yes
Remarks:	In range finding test the correct WAF conc. not specified in protocol, the vortex during WAF formulation did not extend correct distance to bottom of vessel, and daphhid wts could not be verified. Deviations not expected to affect integrity of results.

GLP compliance:	yes

Test material

Test material information

Constituent 1



Reference substance name:	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Pr) esters, zinc salts
EC Number:	272-723-1
EC Name:	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Pr) esters, zinc salts
Cas Number:	68909-93-3
Molecular formula:	Too complex
IUPAC Name:	Phosphorodithioic acid, mixed O,O-bis(2-ethylhexyl and iso-Pr) esters, zinc salts

Details on test material: - Name of test material (as cited in study report): CMA 601

Sampling and analysis

Analytical monitoring:	yes
Details on sampling:	- Concentrations: 0, 1.0, 1.5, 2.5, 5.0, and 6.0 mg/L WAF nominal concentrations

Test solutions

Vehicle:	no
Details on test solutions:	PREPARATION AND APPLICATION OF TEST SOLUTION (especially for difficult test substances) - Method: Each of the five WAFs was prepared by combining the appropriate amount of test substance and dilution water in a glass mixing vessel equipped with a magnetic stirrer (the vortex extended from the surface approximately 30 to 50% of the way to the bottom of the mixing vessel) and stirring these mixtures for approximately 24 hours, settling the mixtures for approximately 1 hour, and siphoning the water phase containing the WAFs. - Eluate: Not applicable - Differential loading: Preparation of test solutions with individually prepared loading rates - Controls: Untreated negative control - Chemical name of vehicle (organic solvent, emulsifier or dispersant): water - Concentration of vehicle in test medium (stock solution and final test solution): Not applicable. - Evidence of undissolved material (e.g. precipitate, surface film, etc):No insoluble material was noted in test vessels containing test substance

Test organisms

Test organisms (species):	Daphnia magna
Details on test organisms:	TEST ORGANISM - Common name: Water Flea - Strain: Daphnia magna - Source: In house laboratory cultures with a known history. The original culture was obtained from Aquatic Research Organisms on May 26, 1992. - Age at study initiation (mean and range, SD): juvenile daphnids less than 24 h old - Weight at study initiation (mean and range, SD): control daphnids had an average wet weight of 0.52 mg at the end of the test - Length at study initiation (length definition, mean, range and SD): no data available. - Valve height at study initiation, for shell deposition study (mean and range, SD): no data available. - Peripheral shell growth removed prior to test initiation: no data available. - Method of breeding: Prior to testing daphnid cultures were maintained in 100% dilution water under static renewal conditions and they were provided with yeast/trout chow and the freshwater alga Selenastrum capricornutum each day - Feeding during test : The daphnids received no food during exposure

- Food type: Not applicable.
- Amount: Not applicable.
- Frequency: Not applicable.

ACCLIMATION
- Acclimation period: from parental daphnids derived from in house laboratory cultures
- Acclimation conditions (same as test or not): Not applicable.
- Type and amount of food: Each culture was fed daily with a suspension of freshwater algae
- Feeding frequency: daily
- Health during acclimation (any mortality observed): The daphnids were free of apparent sickness, injuries and abnormalities at the beginning of the test and there was no mortality in the culture during the 10 days before the start of the test.

QUARANTINE (wild caught)
- Duration: Not applicable.
- Health/mortality: Not applicable.

Study design

Test type:	static
Water media type:	freshwater
Limit test:	no
Total exposure duration:	48 h
Post exposure observation period:	The number of immobilised Daphnia and any adverse reactions to exposure were recorded after 0, 3, 24, and 48 hours

Test conditions

Hardness:	The dilution water had a hardness of 172 mg/L as CaCO3
Test temperature:	The dilution water had a hardness of 172 mg/L as CaCO3
pH:	There were no treatment related differences in pH. pH values ranged from 8.5 to 8.6 at the start of the test, 8.4 after 24 hours, and from 8.2 to 8.3 after 48 hours.
Dissolved oxygen:	There were no treatment related differences in dissolved oxygen concentration (8.3 to 8.8 at start of test, 8.7 to 9.0 after 24 hours, and 8.7 to 9.0 after 48 hours)
Salinity:	not applicable/freshwater
Nominal and measured concentrations:	Nominal loading rates of 0, 1, 1.5, 2.5, 4.0, and 6.0 mg/L WAF.
Details on test conditions:	TEST SYSTEM - Test vessel: 250 mL glass beakers - Type (delete if not applicable): Vessels were loosely covered - Material, size, headspace, fill volume: 250 mL glass vessels containing 200 mL of test solution; water depth was approximately 6 cm. - Aeration: No - Type of flow-through (e.g. peristaltic or proportional diluter): Not applicable. - Renewal rate of test solution (frequency/flow rate): static. - No. of organisms per vessel: 10 per test and control vessel; 20 per concentration No. of vessels per concentration (replicates): duplicate test vessels - No. of vessels per control (replicates): 2 vessels in control - No. of vessels per vehicle control (replicates): Not applicable. - Biomass loading rate: 0.026 g/L in controls at end of test TEST MEDIUM / WATER PARAMETERS - Source/preparation of dilution water: Carbon filtered, dechlorinated tap water collected at TR Wilbury Labs in Marblehead Massachusetts. Water was adjusted to a hardness of 172 mg/L and stored in polyethylene tanks where it was aerated and recirculated through particle filters, activated carbon, and ultraviolet sterilizer. Chemical analysis indicated that the water contained less than 1 ug/L organochlorine pesticides and PCBs. - Total organic carbon: 1.11 mg C/l - Particulate matter: 0.1 mg/L - Metals: NDA - Pesticides: less than 1 ug/L - Chlorine: Dechlorinated - Alkalinity: NDA

- Ca/mg ratio: NDA
- Conductivity: Conductivity in the controls ranged from 630 umhos/cm at the start of the test to 640 after 48 hours.
- Culture medium different from test medium: No difference
- Intervals of water quality measurement: N/A

OTHER TEST CONDITIONS
- Adjustment of pH: NA
- Photoperiod: 16 hours light and 8 hours darkness cycle.
- Light intensity: Cool white fluorescent lights that provided a light intensity of 20 uEin/m2sec.

EFFECT PARAMETERS MEASURED (with observation intervals if applicable) :
Immobilisation, sublethal effects, and survival, recorded initially, after 3 hours, 24 hours, and 48 hours.

TEST CONCENTRATIONS
- Range finding study. The loading rates to be used in the definitive study were determined by a preliminary range finding study.
- Test concentrations: In the range finding study daphnids were exposed to the WAF of 1, 10, and 100 mg/L mixtures of CMA601 and water.
- Results used to determine the conditions for the definitive study: At the conclusion of the exposure 100% of the daphnids exposed to 10 and 100 mg/L WAFs were dead or immobilized and 10% of the daphnids exposed to the 1 mg/L WAF were immobilized

Reference substance (positive control):	not specified

Results and discussion

Effect concentrations

Effect concentrations 1

Duration:	48 h
Dose descriptor:	EC50
Effect conc.:	5.4 mg/L
Nominal / measured:	nominal
Conc. based on:	test mat.
Basis for effect:	mobility
Remarks on result:	other: 4 to 6 mg/L

Effect concentrations 2

Duration:	48 h
Dose descriptor:	NOELR
Effect conc.:	< 1 mg/L
Nominal / measured:	nominal
Conc. based on:	test mat.
Basis for effect:	mobility

Details on results:	- Behavioural abnormalities: NDA - Observations on body length and weight: NDA - Other biological observations: NDA - Mortality of control: 0 - Other adverse effects control: None noted - Abnormal responses: NDA - Any observations (e.g. precipitation) that might cause a difference between measured and nominal values: No insoluble material was noted in test vessels containing CMA 601 throughout the test.
Reported statistics and error estimates:	Results of the toxicity test were interpreted using standard statistical techniques, including the binomial/nonlinear interpolation method

Any other information on results incl. tables

Table 1. Survival Data from the toxicity test with the WAF of 5 concentrations of Test Material and the daphnid, Daphnia magna

	Number of Survivors			
Nominal Concentration WAF (mg/L)	0 hour	3 hour	24 hour	48 hour
0, Control	10	10	10	10
	10	10	10	10
1.0	10	10	10	10
	10	9	9	9
1.5	10	10	10	10
	10	10	10	9
2.5	10	10	10	10
	10	10	10	10
4.0	10	10	10	10
	10	10	10	10
6.0	10	10	10	6
	10	10	10	5

Table 2. Sublethal effect data from the definitive toxicity test with the WAF of 5 concentrations of Test Material and the daphnid, Daphnia magna

	Number Affected			
Nominal Concentration WAF (mg/L)	0 hour	3 hour	24 hour	48 hour
0, Control	0	0	0	0
	0	0	0	0
1.0	0	0	0	0
	0	0	0	0
1.5	0	0	0	0
	0	0	0	0
2.5	0	0	0	4
	0	0	0	1
4.0	0	0	0	0
	0	0	0	0
6.0	0	0	0	1
	0	0	0	5

Justification for Read Across from Analogue EC 272-723-1

Common Manufacturing Process:The submission substance (EC 273-527-9) and the analogue (EC 272-723-1) are produced under a common manufacturing process in which a phosphorodithioic acid ester intermediate, $(RO)_2PS_2H$, is produced by the reaction of phosphorus pentasulfide with an alcohol or a mixture of two alcohols of a similar class - branched alcohol containing C8, C5 and C4 carbons (submission substance) and C3 and C8 carbons (analogue). The intermediate is neutralized with zinc oxide to produce the final multicomponent substance. The reaction is performed in the presence of a highly refined base oil which accounts for 8 – 10.3 % of the final products.

Impurities:The level of impurities in the submission substance and the analogue (data source) is minimal. Impurities have been identified as residual, unreacted alcohols from the production of the phosphorodithioic acid ester intermediates (isobutanol, pentanol and 2-ethylhexanol in the submission substance and isopropanol and 2-ethylhexanol in the analogue).

Same Chemical Category:The submission substance (EC 273-527-9) and the analogue (EC 272-723-1), generically referred to as ZDDPs, have been shown to have sufficient structural similarities to be included in the Zinc Dialkydithiophosphate Category (ZDDPs) in the United States Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program.

Structural Similarity:The primary feature accounting for the similarity of the submission substance (EC 273-527-9) and the analogue (EC 272-723-1) is the common organometallic core structure consisting of a central zinc metal bonded to four alkyldithiophosphate esters (ligands) by coordinate covalent bonds -$Zn[(S_2P(OR)_2]_2$.Structural variations between the submission substance and the analogue are related to the alkyl (R) groups of the alkyldithiophosphate ligands.

The analogue/data source (EC 272-723-1) is a multicomponent mixture of ZDDP monomers and dimers containing isopropyl dithiophosphate ligands, 2-ethylhexyl dithiophosphate ligands, and mixtures of isopropyl and 2-ehtylhexyl dithiophosphate ligands with a molecular weight range of 492 – 772 (monomer).

The submission substance (EC 273-527-9) is a multicomponent mixture of ZDDP monomers and dimers containing isobutyl dithiophosphate ligands, pentyl dithiophosphate ligands, 2-ethylhexyl dithiophosphates ligands and mixtures of isobutyl, pentyl and 2-ethylhexyl dithiophosphate ligands with a molecular weight range of 548 – 772 (monomer).

Tanimoto Fingerprint (ToxMatch Version 1.06 software) gives a similarity index greater than 0.8 (values range from 0, no similarity to 1, identical). Peer reviewed literature indicates that values greater than 0.6 are significantly similar.DSSTox similarity was 80% between the submission substance and the analogue.

Applicant's summary and conclusion

Validity criteria fulfilled:	yes
Conclusions:	The acute toxicity of the test material to the freshwater invertebrate Daphnia magna has been investigated and gave a 48-Hour EC50 value of 5.4 mg/L nominal loading rate with 95% confidence interval from 4 to 6 mg/L. The No Observed Effect Concentration was less than 1 mg/L
Executive summary:	Introduction. A study was performed to assess the acute toxicity of the test material to Daphnia magna. The method followed that described in the OECD Guidelines for Testing of Chemicals No 202, as well as the US CFR Title 40, Part 797, Section 1300. Methods.Following a preliminary range finding study, twenty daphnids (2 replicates of 10 animals) were exposed to Water Accommodated Fractions of the test material over a range of nominal loading rates of 1.0, 1.5, 2.5, 4.0, and 6.0 mg/L. The number of immobilised Daphnia and any adverse reactions to exposure were recorded after 0, 3, 24 and 48 hours. Results.The 48 hour EC50 for the test material to Daphnia magna based on nominal loading rates was 5.4 mg/L with 95% confidence interval from 4 to 6 mg/L. The No Observed Effect Concentration was less than 1 mg/L. Given that toxicity cannot be attributed to a single component or mixture of components but to the test material as a whole, the results were based on nominal loading rates only.