

201-14955A

2-Propenoic Acid, Zinc Salt
(Zinc Acrylate; CAS RN 14643-87-9)

**High Production Volume (HPV) Chemical
Challenge Program Test Plan and Data
Review**

Prepared for:

ACC Specialty Acrylates and Methacrylates Panel

Prepared by:

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December 2003

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Test Plan

2-Propenoic Acid, Zinc Salt (Zinc Acrylate; CAS RN: 14643-87-9)		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL AND CHEMICAL DATA								
2.1	Melting Point	Y	N	Y	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapour Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	Y	N	N	N	Y	N
2.6	Water Solubility	Y	N	N	Y	N	Y	N
ENVIRONMENTAL FATE AND PATHWAY								
3.1.1	Photodegradation	Y	N	N	N	Y	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.3	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	Y	Y	N	N	Y	N
ECOTOXICITY								
4.1	Acute Toxicity to Fish	Y	Y	Y	N	N	Y	N
4.2	Toxicity to Daphnia	Y	Y	Y	N	N	Y	N
4.3	Acute Toxicity to Algae	Y	Y	Y	N	N	Y	N
TOXICITY								
5.1	Acute Toxicity	Y	N	N	Y	N	Y	N
5.4	Repeated Dose Toxicity	Y	Y	Y	Y	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Bacterial Test)	Y	N	N	Y	N	Y	N
5.5	Genotoxicity <i>In Vitro</i> (Mammalian Cells)	Y	Y	N	N	N	Y	N
5.8	Reproductive Toxicity	Y	Y	Y	N	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	Y	Y	N	N	Y	N

**2-Propenoic Acid, Zinc Salt
(Zinc Acrylate; CAS RN 14643-87-9)
High Production Volume Chemical Challenge
Test Plan and Data Review**

1.0 Introduction

This document constitutes a Test Plan and review of available data for the High Production Volume (HPV) Chemical Challenge Program endpoints for 2-Propenoic Acid, Zinc Salt, hereafter called Zinc Acrylate [CAS RN 14643-87-9], for the American Chemistry Council's Specialty Acrylates and Methacrylates Panel.

2.0 General Use and Exposure

Zinc Acrylate (more commonly called zinc diacrylate in the industry) is a monomer used for the production of polymeric materials. It is produced as a powder and is introduced into reaction hoppers with other monomers. The primary use (~ 90%) of Zinc Acrylate is in the production of golf balls. The product serves as a cross-linking agent to produce the rubber core of the ball. Other uses are primarily in the production of specialty rubber products such as belts and hoses for automobiles. In the production plant, local exhaust ventilation is used to help avoid worker contact; extensive monitoring of the production process at manufacturing sites has yet to yield measurable exposure. While dusting occurs from introduction of the product into hoppers during formulation, this process is not done manually and exposure to workers is considered very limited. Because of the nature of the final product (encapsulated polymers) and the extensive cross-linking of the polymer, consumer exposure to Zinc Acrylate is not anticipated.

3.0 Justification for Use of Acrylic Acid Data to Support Zinc Acrylate

Zinc Acrylate is a salt formed from one mole of zinc and two moles of acrylic acid. It is produced as a powder for use in the production of polymers but is water-soluble. The pKa of Zinc Acrylate was determined to be approximately 7.7 in standard tests. Since the chemical is completely water soluble and equilibrium is not reached, complete dissociation occurs in aqueous solutions at the low concentrations that will exist in physiological and environmental exposures. Therefore, the environmental fate and toxicity as well as potential human health toxicity can only be evaluated based on exposure to the dissociation products: zinc and acrylic acid.

The effects of dissociation to acrylic acid are illustrated by tests of Zinc Acrylate in dry and moist conditions. In a primary skin irritation study with six rabbits, only very slight edema was noted in three animals one hour after a four-hour exposure to a Zinc Acrylate formulation containing additives (Cerven, 1991). This minimal effect is consistent with application of dry Zinc Acrylate to skin, where little to no dissociation occurs. However, in an abbreviated eye irritation study in which one rabbit eye was treated with Zinc Acrylate, severe, non-reversible injury occurred following application of a single dose 0.1 ml equivalent of Zinc Acrylate

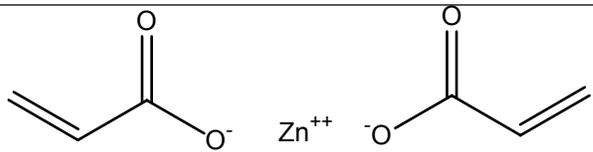
(Moreno, 1993). These effects, observed under the condition of application of Zinc Acrylate in a moist environment, are consistent with exposure to the dissociation product acrylic acid.

Zinc is a metallic element. Metals are not included in the HPV Chemical Challenge Program. Zinc is well studied in humans and is a dietary requirement and is not considered further in this review.

A full European Union (EU) Risk Assessment has been completed on acrylic acid (1st Priority List, Volume 28) and the key studies, as accepted for the Acrylic Acid Risk Assessment, for the HPV Chemical Challenge Program endpoints are summarized in the IUCLID-formatted robust summary file for Zinc Acrylate that accompanies this Test Plan. Zinc Acrylate is not used in the “wet polymerization” types of processes discussed in the EU Risk Assessment for acrylic acid and, therefore, the concerns for the environment identified in the review of acrylic acid do not appear relevant to Zinc Acrylate. For human health, the EU Risk Assessment concluded that no further information or testing was required for consumer exposure or exposure through the environment. Reduction to acrylic acid exposure in workers is required in the acrylic acid assessment only for production of adhesives. Zinc Acrylate is not used in adhesives and, therefore, these concerns do not appear relevant to Zinc Acrylate.

A data summary for Zinc Acrylate is included in Table 1. Table 1 also includes relevant data for acrylic acid.

4.0 General Substance Information (Identity)

Chemical Name	2-Propenoic Acid, Zinc Salt
Synonyms	Zinc Acrylate Zinc Diacrylate 2-Propenoic acid, zinc salt Acrylic acid, zinc salt
CAS Number	14643-87-9
Structure	
Molecular Weight	207.50 (Undissociated Salt)
Substance Type	Organic salt
Physical State	Powder

5.0 Physical/Chemical Properties

A data summary for Zinc Acrylate and acrylic acid is included in Table 1. The Robust Summaries are included in the accompanying IUCLID-formatted file.

5.1 Melting Point

The melting point of Zinc Acrylate was determined using OPPTS Guideline 830.7200. In this test, no obvious liquefaction of the sample occurred in two separate trials, the first continuously heating a single capillary tube and the second heating separate capillary tubes to different temperatures. In the second study, the appearance of the solid Zinc Acrylate changed from white to colorless but did not liquefy. It was concluded that the Zinc Acrylate was undergoing homopolymerization at approximately 235 to 240 °C, a phenomenon known to occur for these types of chemicals in a range of 210 to 240 °C. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

5.2 Boiling Point

Based on the melting point description above, Zinc Acrylate's boiling point is not considered a measurable endpoint. The boiling point of acrylic acid is 141 °C. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

5.3 Vapor Pressure

Based on the physical form and structure, vapor pressure for Zinc Acrylate is of little import. The vapor pressure for the acrylic acid that might be formed during dissociation of Zinc Acrylate is 3.8 hPa at 20 °C. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

5.4 Partition Coefficient

Because Zinc Acrylate is expected to dissociate rapidly to zinc and acrylic acid in environmental water compartments, the log K_{ow} for Zinc Acrylate is considered to provide no useful information for evaluation of environmental fate and effects. The log K_{ow} for acrylic acid is 0.46 indicating a very low potential for bioaccumulation in aquatic organisms. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

5.5 Water Solubility

Zinc Acrylate is expected to dissociate rapidly to zinc and acrylic acid in environmental water compartments. Acrylic acid is miscible with water and, therefore, Zinc Acrylate is also considered to be miscible with water. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

6.0 Environmental Fate

A data summary for Zinc Acrylate and acrylic acid is included in Table 1. The Robust Summaries are included in the accompanying IUCLID-formatted file.

6.1 Photodegradation

The diacrylate salt of zinc could not be modeled using the standard modeling techniques (U.S. EPA, 2000a) used for the HPV Chemical Challenge Program. Because Zinc Acrylate dissociates rapidly in the environment, model data generated for acrylic acid are considered

appropriate for Zinc Acrylate as well. The model prediction for atmospheric photodegradation of acrylic acid provides a second order rate of reaction with hydroxyl radicals of $9.7 \times 10^{-12} \text{ cm}^3/\text{molecule-sec}$ and a $t_{1/2}$ of 13.2 hours (U.S. EPA, 2000a). These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

6.2 Stability in Water

Zinc Acrylate dissociates rapidly to zinc and acrylic acid in environmental water compartments. Acrylic acid has been shown not to hydrolyze at pH 3, 7 or 11 in standard testing (Shah, 1990). Therefore, following dissociation, no hydrolysis of the acrylic acid component of Zinc Acrylate is expected. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

6.3 Transport and Distribution

The diacrylate salt of zinc could not be modeled using the standard modeling techniques (U.S. EPA, 2000b) used for the HPV Chemical Challenge Program. Because Zinc Acrylate is anticipated to dissociate rapidly in the environment, model data generated for acrylic acid are considered appropriate for Zinc Acrylate as well. Environmental exposure to Zinc Acrylate is limited based on the use patterns in enclosed systems and as a cross-linker in final product polymers. Therefore, only unplanned releases were considered for the fugacity modeling. Two scenarios, 100% release to air and 100% release to water were examined. For the air release the model predicted a distribution of 33% into atmosphere, 18% into water, 50% into soil, and < 0.1% into sediment. For the water release the model predicted virtually all of the acrylic acid would remain in the water compartment (99.8%). These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

6.4 Biodegradability

Zinc Acrylate dissociates rapidly to zinc and acrylic acid in environmental water compartments. Acrylic acid has been shown to degrade rapidly in an OECD 301D test (81% in 28 days meeting the “10-day window”) and is considered readily biodegradable (Douglas, 1991). Therefore, Zinc Acrylate is also considered to undergo rapid biodegradation in the environment. These data are considered adequate to meet the HPV Chemical Challenge Program requirements.

7.0 Ecotoxicity

A data summary for Zinc Acrylate and acrylic acid is included in Table 1. The robust summaries are included in the accompanying IUCLID-formatted file.

7.1 Toxicity to Fish

Since Zinc Acrylate dissociates rapidly to zinc and acrylic acid in the environment, the LC_{50} value for acrylic acid of 27 mg/L for rainbow trout (Bowman, 1990) is considered appropriate for the evaluation of the potential toxicity of Zinc Acrylate to fish. These data are considered adequate to meet HPV Chemical Challenge Program requirements.

7.2 Toxicity to Aquatic Invertebrates

Because Zinc Acrylate dissociates rapidly to zinc and acrylic acid in the environment, the EC₅₀ value for acrylic acid of 47 mg/L for *Daphnia magna* (Huels, 1995a) is considered appropriate for the evaluation of the potential toxicity of Zinc Acrylate to invertebrate species. In addition, a study evaluating the effect of acrylic acid on reproduction in *Daphnia magna* provided a NOEC for reproduction rate of 12 mg/L (Huels, 1995b). These data are considered adequate to meet HPV Chemical Challenge Program requirements.

7.3 Toxicity to Aquatic Plants

Since Zinc Acrylate dissociates rapidly to zinc and acrylic acid in the environment, the EC₅₀ value for acrylic acid of 0.04 mg/L for green algae, *Scenedesmus subspicatus* (BASF, 1994), is considered appropriate for the evaluation of the potential toxicity of Zinc Acrylate to aquatic plants. These data are considered adequate to meet HPV Chemical Challenge Program requirements.

8.0 Human Health-Related Data

A data summary for Zinc Acrylate and acrylic acid is included in Table 1. The robust summaries are included in the accompanying IUCLID-formatted file. As noted in Section 3.0, the studies summarized below and in the robust summaries are for acrylic acid.

8.1 Acute Toxicity

The acute oral LD₅₀ in rats for acrylic acid is 1337 mg/kg bw (Dow, 1992). This value is considered adequate to meet the HPV Chemical Challenge requirements. The acute dermal LD₅₀ in rabbits for acrylic acid is 640 mg/kg bw (BASF, 1979).

8.2 Repeated Dose Toxicity

Two drinking water studies with rats (BASF, 1987; Inter-Company Acrylate Study Group, 1980) and inhalation studies with rats and mice (Dow, 1979) of at least 90 days duration are available for acrylic acid. The primary effects observed in these studies are related to the irritant properties of acrylic acid or responses most likely related to reduced water consumption or irritant properties. No specific organ toxicity, other than for irritation at the site of contact, was observed in any of these 90-day studies although some organ weights were altered, particularly kidney, in the drinking water studies that was likely related to reduced water consumption. Overall, these studies indicate that Zinc Acrylate would not be expected to exhibit significant toxicity at exposures far in excess of those that might occur from accidental ingestion or contact with the chemical. The available data are considered adequate to meet HPV Chemical Challenge Program requirements.

8.3 Genetic Toxicity

8.3.1 *In vitro*

Zinc Acrylate was tested in a bacterial gene mutation assay with Salmonella strains TA-1535, TA1537, TA-1538, TA-98 and TA-100. Zinc Acrylate was negative with and without metabolic activation at concentrations ranging from 0.1 to 500 µg/plate (Jagannath, 1977).

A series of *in vitro* mutagenicity assays conducted according to OECD guidelines are available for acrylic acid. Bacterial gene mutation (Cameron *et al.*, 1991) and mammalian (HGPRT) cell (McCarthy *et al.*, 1992) assays were negative. A positive response was observed in a cytogenetic assay (McCarthy *et al.*, 1992) as well as in a mouse lymphoma assay (Cameron *et al.*, 1991). Similar results to those observed in these latter two studies have been noted for some esters of acrylic acid. In general, these responses occur in the presence of cytotoxicity. It has previously been noted that there is an association between chromosomal aberrations and cytotoxicity at exposure concentrations that reduce cell growth to less than 50% of the control value (Galloway, 2000 and references cited therein). The Acrylic Acid Risk Assessment concluded that, in light of all available data, it is unlikely that acrylic acid is mutagenic *in vivo* and a similar conclusion is drawn for Zinc Acrylate. The available data are considered adequate to meet HPV Chemical Challenge Program requirements.

8.4 Reproductive and Developmental Toxicity

A two-generation reproduction study with acrylic acid in drinking water conducted according to OECD Guideline 416 is available (BASF AG, 1994). No effects on reproductive parameters or fertility were observed at 5000 ppm acrylic acid (highest dose tested) in the drinking water. Some toxicity to the dams and retarded growth and development of the offspring were observed at 2500 and 5000 ppm. A developmental toxicity study in rats (Klimisch and Hellwig, 1991) and a second study in rabbits (Union Carbide, 1993) via inhalation conducted according to OECD Guideline 414 are available for acrylic acid. In the rat study, maternal toxicity was observed at all concentrations (40, 120, and 360 ppm; 0.12, 0.36 and 1.08 mg/L). In the rabbit study, maternal toxicity was observed at 75 and 225 ppm (0.225 and 0.675 mg/L) but not at the lowest concentration of 25 ppm (0.075 mg/L). No effects on development and no terata were observed in either study. Acrylic acid and Zinc Acrylate are not considered to be reproductive or developmental toxicants based on available information. The available data are considered adequate to meet HPV Chemical Challenge Program requirements.

9.0 Conclusion

Zinc Acrylate is a salt that dissociates rapidly to zinc and acrylic acid. Therefore, the data for acrylic acid have been used extensively in evaluation of HPV/SIDS endpoints. An attempt to measure the melting point of Zinc Acrylate indicated that the chemical will not melt but rather homopolymerizes near the melting point temperature. Adequate information is available for boiling point, vapor pressure and partition coefficient for acrylic acid and, therefore, Zinc Acrylate. Photodegradation and environmental distributions are adequately supported by the appropriate model data for acrylic acid. Zinc acrylate, as a salt, is completely water soluble and following dissociation to acrylic acid, hydrolysis will not occur. Since Zinc Acrylate will completely dissociate at concentrations that could accidentally occur in the environment, the aquatic tests with fish, invertebrates and plants, for acrylic acid adequately support the potential environmental toxicity of Zinc Acrylate. Acrylic acid rapidly degrades in the environment and, therefore, Zinc Acrylate is biodegradable. Acute and subchronic toxicity evaluations of acrylic acid are adequate to support the evaluation of potential toxicity of Zinc Acrylate and indicate that

the primary concern is related to the site of contact and the resulting irritant effects. In bacterial and mammalian cell systems Zinc Acrylate and acrylic acid are negative for mutagenic activity. Although acrylic acid, as well as several esters of acrylic acid, show positive responses in mammalian cell mutagenicity assays, these responses occur only in the presence of significant cellular toxicity. Overall, in agreement with the Acrylic Acid Risk Assessment, in light of all available data, it is unlikely that acrylic acid and Zinc Acrylate are mutagenic *in vivo*. As with repeated dose studies, evaluation of the reproductive and developmental toxicity of acrylic acid is adequate for Zinc Acrylate and confirm that Zinc Acrylate does not affect reproduction or the developing offspring. Overall, the available data for acrylic acid, consistent with the conclusions of the EU Risk Assessment, and Zinc Acrylate are considered adequate to meet the HPV Chemical Challenge Program requirements.

10.0 References

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Table 1: HPV Data Summary
2-Propenoic Acid, Zinc Salt

CAS NO: 14643-87-9		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point		OPPTS 830.7200 – for Zinc Acrylate	Homopolymerization at 235 – 240 °C (see Robust Summary)
2.2	Boiling Point		Handbook Data (CRC) – for Acrylic Acid	141 °C
2.4	Vapor Pressure		Company information – for Acrylic Acid	3.8 hPa (at 20 °C)
2.5	Partition Coefficient (log K _{ow})		OECD 107 – for Acrylic Acid	0.46
2.6	Water Solubility		Handbook Data (CRC) – for Acrylic Acid	Miscible – Infinitely soluble
2.12	Dissociation Constant		OPPTS 830.7370 – for Zinc Acrylate	7.71 – see Text
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation		AOPWIN v. 1.91 – for Acrylic Acid	half-life: 13.2 hours (OH Rate Constant)
3.1.2	Stability in Water		Not Specified – for Acrylic Acid	No hydrolysis at ph 3, 7 or 11 over 28 days
3.3	Transport and Distribution		Mackay Level III – for Acrylic Acid 100% release to air – for Acrylic Acid	33% into atmosphere, 18% into water, 50% into soil, < 0.1% into sediment
			Mackay Level III – for Acrylic Acid 100% release to water – for Acrylic Acid	< 0.01% into atmosphere, 99.8% into water, < 0.1% into soil, < 1% into sediment
3.5	Biodegradation		OECD 301D – for Acrylic Acid	81% after 28 days; Acrylic Acid Readily Biodegradable
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish*	<i>Salmo gairdneri</i>	OECD 203 – for Acrylic Acid	LC ₅₀ (96 hours) = 27 mg/L
4.2	Acute Toxicity to Aquatic Invertebrates*	<i>Daphnia magna</i>	Directive 92/69/EEC, C.2 – for Acrylic Acid	EC ₅₀ (48 hours) = 47 mg/L
4.3	Toxicity to Aquatic Plants e.g. Algae*	<i>Scenedesmus subspicatus</i>	EC Guideline 79/831/EEC, Annex V, C, 1988 – for Acrylic Acid	EC ₅₀ (72 hours) = 0.04 mg/L

Table 1: HPV Data Summary				
2-Propenoic Acid, Zinc Salt				
CAS NO: 14643-87-9		SPECIES	PROTOCOL	RESULTS
4.5.2	Chronic Toxicity to Aquatic Invertebrates	<i>Daphnia magna</i>	OECD 202, part 2 – for Acrylic Acid	NOEC (Reproduction rate) = 12 mg/L
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	Not specified – for Acrylic Acid	LD ₅₀ : 1337 mg/kg bw
5.1.3	Acute Dermal Toxicity	Rabbit	Not specified – for Acrylic Acid	LD ₅₀ : 640 mg/kg bw
5.4	Repeated Dose Toxicity	Rat	OECD 408 – Drinking water (120, 800, 2000, 5000 ppm) – for Acrylic Acid	NOAEL = 800 ppm (40 – 66 mg/kg/day)
	Repeated Dose Toxicity	Rat	Not specified – Drinking water (83, 250, 750 mg/kg/day) – for Acrylic Acid	NOAEL = 83 mg/kg/day
	Repeated Dose Toxicity	Rat	Similar to OECD 413 – Inhalation (5, 25, 75 ppm) – for Acrylic Acid	NOAEL = 25 ppm (0.074 mg/L)
	Repeated Dose Toxicity	Mouse	OECD 413 – Inhalation (5, 25, 75 ppm) – for Acrylic Acid	NOAEL = Not established
5.5	Genetic Toxicity <i>In Vitro</i> Bacterial Test (Gene mutation)	<i>Salmonella typhimurium</i>	Ames – for Zinc Acrylic	Negative
		<i>Salmonella typhimurium</i>	OECD 471 – for Acrylic Acid	Negative
		CHO: Chromosomal Aberration	OECD 473 – for Acrylic Acid	Positive
		CHO: HGPRT	OECD 476 – for Acrylic Acid	Negative
		Mouse lymphoma	OECD 476 – for Acrylic Acid	Positive
	Rat hepatocyte - UDS	OECD 482 – for Acrylic Acid	Negative	

Table 1: HPV Data Summary				
2-Propenoic Acid, Zinc Salt				
CAS NO: 14643-87-9		SPECIES	PROTOCOL	RESULTS
TOXICOLOGY (continued)				
5.8	Toxicity to Reproduction / Impairment of Fertility	Rat	OECD 416 – Drinking water (500, 2500, 5000 ppm) – for Acrylic Acid	NOAEL (Reproduction) = 5000 ppm (460 mg/kg/day)
5.9	Developmental Toxicity / Teratogenicity	Rat	OECD 414 – Inhalation (40, 120, 360 ppm) – for Acrylic Acid	NOAEL (Maternal toxicity) < 40 ppm (0.12 mg/L) NOAEL (Embryo-fetal toxicity) = 360 ppm (1.08 mg/L)
		Rabbit	OECD 414 – Inhalation (25, 75, 225 ppm) – for Acrylic Acid	NOAEL (Maternal toxicity) = 25 ppm (0.075 mg/L) NOAEL (Embryo-fetal toxicity) = 225 ppm (0.675 mg/L)