201-14923A

HIGH PRODUCTION VOLUME (HPV)

CHALLENGE PROGRAM

TEST PLAN

For

Benzoic Acid, 2-Hydroxy-, Mono-C14-18 Alkyl Derivatives, Calcium Salts

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group

December 2003

LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel include the following member companies:

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

ExxonMobil Chemical Company

Ferro Corporation

Groupe SNPE

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc.

1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment. Specifically, this test plan sets forth how the HERTG intends to address testing information for the following substance - Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts (CAS No.: 114959-46-5).

In preparing this test plan the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physicochemical properties, mammalian toxicity endpoints, and environmental fate and effects for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts, using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physicochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

2.0 GENERAL SUBSTANCE INFORMATION

The substance that is the subject of this test plan is used as a petroleum additive in highly refined lubricant base oil . The chemical name, CAS Registry Number, molecular weight and chemical structure for this substance are presented below.

Chemical Name: Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts

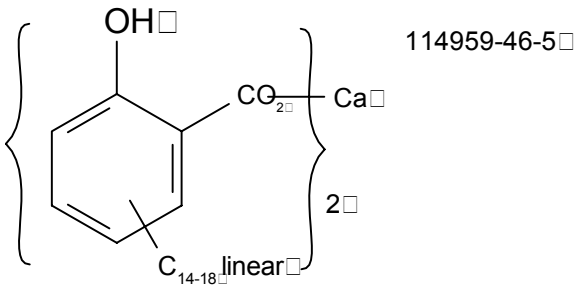
Chemical Abstract Service Registry Number: 114959-46-5

Molecular Weight: 765 gm/mole (Based on average olefin chain length of C16).

Testing was previously conducted on the substance using two formulations of benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts. One formulation was 43% benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts, 48% highly refined lubricating base oil and 9% inorganic calcium salts; this formulation will be referred to in the test plan as “AI-43”. The second formulation was 28% benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts, 51% highly refined lubricating base oil and 21% inorganic calcium salts; this formulation will be referred to in the test plan as “AI-28”.

In the general discussion of manufacture and use, the material will be referred to as calcium alkyl salicylates.

Chemical Structure:



3.0 EXPOSURE INFORMATION

Manufacture

Calcium alkyl salicylates are manufactured as described below:

Alkyl phenol is produced by the reaction of phenol with long chain olefins (C14-C18). The refined alkyl phenol is diluted with xylene and then reacted with caustic soda (sodium hydroxide) to form sodium alkyl phenate. The phenate salt is converted to sodium alkyl salicylate (carboxylate) by reaction with carbon dioxide. The carboxylate is then reacted with sulphuric acid (diluted in water) to give alkylsalicylic acid.

The component under review, a calcium alkyl salicylate, is produced by neutralisation of alkylsalicylic acid with calcium hydroxide (lime) and carbonation in the presence of methanol.

Excess solids and solvents are then removed by solid separation and solvent stripping.

Use

Calcium alkyl salicylates are detergent additives used in gasoline and diesel engine oils. Additional functionality includes excess basicity for neutralisation of acids, detergency to assist in keeping carbon particles (soot) in suspension and minimising sludge formation, and to act as anti-oxidant and anti-rust preventative agents.

4.0 PHYSICOCHEMICAL PROPERTIES

4.1 Summary of Available Data

Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts has a water solubility of >9mg/L and a log octanol/water partition coefficient of >3.9. There were no other physical/chemical properties data located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

4.2 Data Assessment and Test Plan for Physicochemical Properties Relevant to Environmental Fate

Adequate and reliable water solubility and n-octanol/water partition coefficient data are available for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts. Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts is a liquid at ambient temperatures (thus melting point is not applicable). No published or unpublished data were located for boiling point or vapor pressure. These parameters will be evaluated using AI-43.

5.0 ENVIRONMENTAL FATE DATA

5.1 Biodegradability

5.1.1 Summary of Available Data

AI-43 exhibited biodegradation of 39% at 28 days and 63% at 56 days.

5.1.2 Data Assessment and Test Plan for Biodegradability

An adequate and reliable biodegradation study has been conducted on benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts. The results indicate that this material is inherently biodegradable. Additional biodegradation testing is not proposed.

5.2 Hydrolysis

5.2.1 Summary of Available Data

No adequate published or unpublished hydrolysis studies were located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

5.2.2 Data Assessment and Test Plan for Hydrolysis

Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts does not contain any readily hydrolysable functional groups, therefore, no hydrolysis testing is planned.

5.3 Photodegradation

5.3.1 Summary of Available Data

No adequate published or unpublished photodegradation studies were located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

5.3.2 Data Assessment and Test Plan for Photodegradation

A technical discussion will be developed to characterize the photodegradation of this material.

5.4 Fugacity Modeling

5.4.1 Summary of Available Data

No adequate published or unpublished fugacity-based multimedia fate modeling data were located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

5.4.2 Test Plan for Fugacity

The relative distribution of benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts among environmental compartments will be evaluated using Level I Fugacity modeling.

Input data to run the EQC Level I model will require an additional computer model to estimate physical/chemical properties from a structure. The model used for this purpose will be EPIWIN, version 3.02[1], which was developed by the Syracuse Research Corporation. EPIWIN includes algorithms for estimating all physical and chemical properties needed for the EQC model.

6.0 ECOTOXICOLOGY DATA

6.1 Aquatic Ecotoxicity Testing

6.1.1 Summary of Available Data

Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts was evaluated for acute toxicity in freshwater fish, for acute and chronic toxicity in *Daphnia magna*, and for acute toxicity in freshwater algae (*Pseudokirchneriella subcapitata*).

Rainbow trout were tested by exposing them to a WAF prepared at loadings of 0, 220, 460 and 1000 mg/L of AI-28. No mortality was observed at 24, 48, 72 or 96 hours for any of the test concentrations. Therefore, the 96-hour LL_{50} was > 1000 mg/L WAF.

In an acute *Daphnia magna* toxicity study with AI-43, 100% immobilization occurred at ≥100 mg/L (WAF) at 48 hours and at 1000 mg/L at 24 hours. The no observed effect level was 10 mg/L (WAF). Therefore, the 48 hour EL50 was between 10 and 100 mg/L. In an acute *Daphnia magna* toxicity study with AI-28, no immobilizations were observed using WAF preparations of 0, 100, 220, 460 and 1000 mg/L. Therefore, the 48 hour EL50 was >1000 mg/L and the NOEC was 1000 mg/L. In a chronic toxicity study with AI-43, mortality was higher than controls in *Daphnia magna* exposed to 1 mg/L (WAF) for 21 days. However, the reproductive performance of the surviving daphnids was not significantly affected compared to control animals.

The 48-96 hour EL50 of AI-43 in freshwater algae (*Pseudokirchneriella subcapitata*) was > 1000 mg/L (WAF). The 0-72 hour EL50 of AI-28 in freshwater algae (*Pseudokirchneriella subcapitata*) was > 1000 mg/L (WAF).

6.1.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity

[1] Environmental Science Center- Syracuse Research Corporation- EPI for windows.

The available acute toxicity data in freshwater fish, the acute and chronic toxicity data in *Daphnia magna*, and the acute toxicity data in freshwater algae are adequate and reliable. Additional acute or chronic aquatic ecotoxicity testing will not be conducted.

7.0 MAMMALIAN TOXICOLOGY DATA

7.1 Acute Mammalian Toxicity

7.1.1 Summary of Available Data

Acute oral and dermal toxicity studies are available for AI-28. In these studies, the LD50s were greater than 5000 mg/kg by the oral route and greater than 2000 mg/kg by the dermal route indicating a low concern for toxicity.

7.1.2 Data Assessment and Test Plan for Acute Mammalian Toxicity

Adequate and reliable acute oral and dermal toxicity tests are available for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts. Additional acute mammalian toxicity testing will not be conducted.

7.2. Mutagenicity

7.2.1 Summary of Mutagenicity Data

Both AI-43 and AI-28 were non-mutagenic in *Salmonella typhimurium* and *Escherichia coli* in vitro point mutation assays. No adequate published or unpublished chromosomal aberration testing was located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

7.2.2 Data Assessment and Test Plan for Mutagenicity Toxicity

Adequate and reliable *Salmonella typhimurium* and *Escherichia coli* in vitro point mutation assays are available for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts. In vitro chromosomal aberration testing of AI-43 will be conducted.

7.3 Repeated-dose, Reproductive and Developmental Toxicity

7.3.1 Summary of Repeated-Dose Toxicity Data

No adequate published or unpublished repeat dose, reproductive or developmental toxicity studies were located for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

7.3.2 Data Assessment and Test Plan for Repeated-dose Toxicity

Repeated dose toxicity and reproductive/developmental toxicity will be evaluated for benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

8.0 SUMMARY

The following table summarizes the available data and proposed testing on benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts.

Table 1: Summary Table of Available Data and Proposed Testing

	Testing Proposed	**Study Results**	
	114959-46-5	**Test Campaign 1**	**Test Campaign 2**
	Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts	AI-43	AI-28
Physical/Chemical Characteristics			
Melting Point	Not Applicable	Not Applicable	Not Applicable
Boiling Point	Yes	No Adequate Data Located	No Adequate Data Located
Vapor Pressure	Yes	No Adequate Data Located	No Adequate Data Located
Water Solubility	No	9 mg/L (0.9 – 90 mg/L)	30±16 mg/L at 1 g/L loading rate 103±6 mg/L at 100 g/L loading rate
Partition Coefficient	No	Log P_{ow} >3.9	No Adequate Data Located
Environmental Fate			
Biodegradation	No	39% at 28 days 63% at 56 days	No Adequate Data Located
Hydrolysis	Not Applicable	No Adequate Data Located	No Adequate Data Located
Photodegradation	Technical Discussion	No Adequate Data Located	No Adequate Data Located
Fugacity	Modeling	No Adequate Data Located	No Adequate Data Located

Table 1: Summary Table of Available Data and Proposed Testing (continued)

	Testing Proposed	Study Results	
	114959-46-5	**Test Campaign 1**	**Test Campaign 2**
	Benzoic acid, 2-hydroxy-, mono-C14-18 alkyl derivatives, calcium salts	AI-43	AI-28
Ecotoxicity			
Acute Toxicity to Fish	No	No Adequate Data Located	96 hour LL50 >1000 mg/L (WAF) 96 hour NOEC: 1000 mg/L (WAF)
Acute and Chronic Toxicity to Invertebrates	No	Acute Toxicity: 48 hour EL50 between 10-100 mg/L, 100% immobilization at ≥ 100 mg/L (WAF); NOEL = 10 mg/L (WAF) Chronic Toxicity: 1 mg/L (WAF) for 21 days; Mortality higher than controls; No effect on reproduction	48 hour EL50 > 1000 mg/L (WAF) 48 hour NOEC: 1000 mg/L (WAF)
Acute Toxicity to Algae	No	48-96 hour EL50 > 1000 mg/L (WAF)	0-72 hour EL50 > 1000 mg/L (WAF)
Mammalian Toxicity			
Acute Toxicity	No	No Adequate Data Located	Oral LD50 >5000 mg/kg Dermal LD50 >2000 mg/kg
Repeated Dose Toxicity	Yes	No Adequate Data Located	No Adequate Data Located
Developmental Toxicity	Yes	No Adequate Data Located	No Adequate Data Located
Reproductive Toxicity	Yes	No Adequate Data Located	No Adequate Data Located
Genotoxicity			
Gene Mutation	No	Not Mutagenic	Not Mutagenic
Chromosomal Aberration	Yes	No Adequate Data Located	No Adequate Data Located