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HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

-

TEST PLAN

For

9-Octadecenoic Acid (Z)-Cobalt Salt

Prepared by:

ExxonMobil Chemical Company

Date: November 28, 2006

EXECUTIVE SUMMARY

Under the U.S. Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company (EMCC) committed to voluntarily compile data that can be used in an initial assessment to characterize the hazard of 9-octadecenoic acid (Z)-cobalt salt (cobalt oleate; CAS No. 14666-94-5). The data for this assessment include selected physicochemical, environmental fate, and human and environmental effect endpoints identified by the U.S. HPV Program.

A search for existing studies and their review identified limited data for cobalt oleate to characterize all endpoints. However, data exist for octadecanoic acid-cobalt salt (cobalt stearate; CAS No. 13586-84-0) and fatty acids, tall oil, cobalt salt (CAS No. 61789-52-4), which are structurally similar to the EMCC substance, with the latter possessing a carbon-carbon double bond at the 9 position. Metal carboxylates such as cobalt oleate; cobalt stearate; and fatty acids, tall oil, cobalt salt can dissociate to the corresponding cobalt and carboxylic acid(s). Data for the dissociation products, cobalt and oleic acid are also available, and employed for both mammalian and environmental endpoints as read-across data in this test plan. Data for tall oil fatty acid, of which oleic acid is a major component, are also employed as read-across data in this test plan.

Data for cobalt stearate and the dissociation products of cobalt oleate suggest that cobalt oleate generally presents a low to moderate order of hazard for human health. Additional supporting data will be collected for another HPV testing program for substances similar in structure to cobalt oleate. These data are expected to provide sufficient information to develop scientific judgment-based characterizations of the human health effects of cobalt oleate for purposes of satisfying HPV program requirements.

Data for the dissociation products of cobalt oleate suggests that this compound will have a low to moderate hazard to environmental health, generally via the cobalt dissociation product. Additional supporting data for a structural analog of cobalt oleate will be collected for another HPV testing program. These data, accompanied by existing data will provide sufficient information to develop a scientific judgment-based characterization of the environmental effects of cobalt oleate for the purpose of satisfying HPV program requirements.

TABLE OF CONTENTS

Cobalt Oleate

I. INTRODUCTION

Under the U.S. Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company committed to voluntarily compile data for 9-octadecenoic acid (Z)-cobalt salt (cobalt oleate; CAS No. 14666-94-5).

This substance is supported by selected screening data needed for an initial assessment of physicochemical properties, environmental fate, and human and environmental effects as identified by the U.S. HPV Program.

Procedures to assess the reliability of selected data for inclusion in this test plan were based on guidelines described by Klimisch *et al*., (1997) (Appendix A) and identified within the US EPA (1999a) document titled Determining the Adequacy of Existing Data.

II. CHEMICAL PROCESS AND DESCRIPTION

For purposes of the HPV Program, the chemical name is cobalt oleate (CAS No. 14666-94-5). This substance is a catalyst used in the production of oxo alcohols. Although the form of the cobalt changes in the reaction process, it is recovered and recycled on-site in a sustainable manner to produce more cobalt oleate. Neither cobalt oleate nor any of the cobalt reaction co-products are manufactured for sale or leave the production site.

Cobalt oleate is a metal carboxylate salt represented by the following chemical formulas:

$Co(C_{18}H_{33}O_2)_2$ $C_{18}H_{33}O_2(Co)C_{18}H_{33}O_2$

III. TEST PLAN RATIONALE AND DATA SUMMARY

Data used to characterize the physicochemical, mammalian and environmental toxicity, and environmental fate endpoints in the HPV Program are described below.

A literature search for mammalian and environmental toxicity data for cobalt oleate did not identify measured data. However, adequate read-across data are available for the dissociation products of cobalt oleate: the cobalt ion, and oleic acid. Additional data were identified for cobalt stearate; and fatty acids, tall oil, cobalt salt. These two compounds have been submitted in an HPV Test Plan prepared by the Synthetic Organic Chemical Manufacturers Association (SOCMA) Metal Carboxylates Coalition. Both are similar to in structure to cobalt oleate. Cobalt stearate is the unsaturated C18 carboxylate, while tall oil, fatty acids, cobalt salt is a mixture of fatty acid carboxylates of which cobalt oleate is a major component. As with the SOCMA HPV Test Plan, an appropriate assessment for cobalt oleate must consider the potential of this compound to dissociate to form cobalt and oleic acid under aqueous conditions.

As such, data for the dissociation products (cobalt and oleic acid) are recognized as being useful in understanding the human and environmental health hazards and environmental effects of cobalt oleate. The work described in the HPV test plan prepared by the SOCMA Metal Carboxylates Coalition (2005) shows that cobalt chloride is similar to, or more bioavailable than, the corresponding cobalt carboxylate salt, which makes cobalt chloride a conservative surrogate in estimating the toxicity of dissociated

cobalt. In addition, it has been demonstrated that absorption, distribution, and excretion of cobalt from cobalt carboxylates is independent of the carboxylic acids (Metal Carboxylates Coalition, 2005).

A. Physicochemical Data

Physicochemical data (Table 1) were not identified for cobalt oleate, thus calculated data are provided from the Estimation Programs Interface Suite (EPISuite™, 2004), as discussed in the EPA document titled The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program (U.S. EPA, 1999b). Measured data for analogs cobalt stearate and fatty acids, tall oil, cobalt salt (Metal Carboxylates Coalition, 2005), are included as read-across data for reference purposes. Boiling point data was not included for cobalt stearate, as this compound was reported to decompose before reaching the boiling point (Metal Carboxylates Coalition, 2005). A boiling point was not achieved for tall oil, fatty acids, cobalt salt (Metal Carboxylates Coalition, 2005). The octanol-water partition coefficient (K_{OW}) was deemed an appropriate property to measure for cobalt stearate, and tall oil, fatty acids, cobalt salt as these compounds do not constitute unionized, undissociated chemicals (Metal Carboxylates Coalition, 2005). Data for oleic acid were supplied by the database of experimental values contained within the EPI Suite model.

Table 1. Selected Physicochemical Properties for Cobalt Oleate

DATA SOURCE	MELTING POINT (º C)	BOILING POINT (º C)	VAPOR PRESSURE (Pa)	WATER SOLUBILITY (mg/L)	LOG K_{ow}
Calculated (cobalt oleate)	313.2	668.2	1.7×10^{-13}	3.2×10^{-11}	14.71
Analog* (cobalt stearate)	45.5 to 79.3	ND	-	6.4 (20 °C)	-
Analog* (fatty acids, tall oils, cobalt salt	-38 to -39	ND	-	149 (20 °C)	-
Oleic acid**	13.4 (m)	360 (m)	1.9×10^{-4} (c)	0.01 (c)	7.64 (m)

ND No data

* Data obtained from the Pine Chemicals Association through the SOCMA Metal Carboxylates Coalition HPV test plan for cobalt stearate and fatty acids, tall oil, cobalt salts

** Data obtained as measured (m) or calculated (c) from the EPISuite (2004) database

B. Human Health Effects Data

Data for a structurally similar substance (cobalt stearate) and dissociation products (cobalt and oleic acid) are available to characterize the potential human health hazards of cobalt oleate. Except for cobalt (as cobalt chloride), the available data demonstrated a low order of acute toxicity by the oral and dermal routes of exposure. *In vitro* genotoxicity testing indicated no evidence of mutagenic activity in point mutation assays with and without metabolic activation using *Salmonella typhimurium* strains with

dissociation products. Cobalt chloride produced a concentration-dependent increase in total chromosomal aberrations in an *in vivo* mouse micronucleus assay. A low to moderate order of toxicity was observed in subchronic dietary testing with dissociation products. Reproductive effects were noted in male and female rats exposed to cobalt chloride and oleic acid, respectively. Additional data on mammalian health effects of the structural analog, cobalt stearate will be available by other HPV testing program to fill data gaps.

Acute Toxicity

Data for a structurally similar substance (cobalt stearate) and dissociation products (cobalt and oleic acid) are available to characterize the potential acute toxicity of cobalt oleate. The oral rat LD_{50} values for cobalt stearate, cobalt and oleic acid were 9820 mg/kg (Metal Carboxylates Coalition, 2005), 42.4 – 190 mg/kg (Metal Carboxylates Coalition, 2005) and >21.5 mL/kg (CIR, 1987), respectively. The dermal LD_{50} value for oleic were >3000 mg/kg (CIR, 1987). Due to the low vapor pressure resulting in a low level of maximal attainable vapor concentration, inhalation exposure is expected to pose a negligible hazard. Thus, for purposes of the HPV Challenge Program, the available data on a structurally similar substance and dissociation products is adequate to characterize the acute toxicity of the cobalt oleate. Therefore, no additional testing for acute toxicity is proposed.

Genotoxicity

Studies have been conducted to evaluate the mutagenic activity of the dissociation products of cobalt oleate. In bacterial reverse gene mutation assays with and without metabolic activation, cobalt (as cobalt chloride) and oleic acid demonstrated no mutagenic activity in S*almonella typhimurium* strains (Metal Carboxylates Coalition, 2005; Mortelmans *et al.*, 1986).

The clastogenicity of cobalt (as cobalt chloride) was tested in an *in vivo* mouse micronucleus assay. Cobalt chloride produced a concentration-dependent increase in total chromosomal aberrations (Metal Carboxylates Coalition, 2005).

Available data for the dissociation products allow use of scientific judgment to characterize the potential of cobalt oleate to cause genotoxicity. In addition, chromosomal aberration data for the structural analog of cobalt oleate are under development by the Synthetic Organic Chemical Manufacturers Association Metal Carboxylates Coalition under the HPV program (see Table 2). Thus, no additional testing for genotoxicity is proposed.

Repeated Dose Toxicity

A repeated oral dosing of rats with cobalt chloride at levels ranging from 0.5 to 30.2 mg Co/kg/day for periods ranging from 12-16 days up to 7 months resulted in reduced weight gain, increases in some organ weights (heart, liver and lungs), increased hematocrit, hemoglobin, and red blood cells, renal tubular necrosis, and various changes on cardiac physiology (left ventricular hypertrophy, impaired ventricular function, and degeneration of myofibrils). The neurotoxic effects of cobalt have been also reported in rats after chronic dietary exposures. The No Observed Adverse Effect Level (NOAEL) was determined to be 0.6 mg Co/kg/day (Metal Carboxylates Coalition, 2005).

Feeding diets containing 15% oleic acid to rats for 10-16 weeks had no adverse effects on growth or general health except for the reproductive capacity of females. No lesions in non-reproductive organs were observed. A few rats had ovarian cysts (Carroll and Noble, 1957).

Available data for dissociation products allow use of scientific judgment to characterize the potential of the cobalt oleate to cause repeated dose toxicity. In addition, data from combined repeated dose with reproduction/developmental toxicity screening test (OECD 422) with the structural analog of cobalt oleate are under development by the Synthetic Organic Chemical Manufacturers Association Metal Carboxylates Coalition under the HPV program (see Table 2). Thus, no additional testing for genotoxicity is proposed.

Developmental and Reproductive Toxicity

Multiple developmental and reproductive toxicity studies have been conducted on cobalt chloride (Metal Carboxylates Coalition, 2005).

Pregnant rats were dosed daily with 25, 50 or 100 mg/kg cobalt chloride (equivalent to 6.2, 12.4 and 24.8 mg Co/kg) by oral gavage during gestation days 6 to 15. On day 20 of gestation, dams were weighed, and then sacrificed. After exsanguinations the uterine horns were opened and number of corpora lutea, total implantations, live and dead fetuses, fetal body length, and fetal tail length were examined. Fetuses were also fixed, stained and examined for skeletal abnormalities. Maternal effects included significant reductions in weight gain and food consumption, and increases in hematocrit and hemoglobin contents at the highest dose. No treatment-related changes were observed in the number of corpora lutea, total implants, resorptions, number of live and dead fetuses per litter, fetal size parameters, or fetal sex ratio. Examination of fetuses for gross external abnormalities, skeletal malformations, and ossification variations indicated no teratogenicity or significant fetotoxicity in the rat. Based on these results, the NOAEL was 12.4 mg Co/kg/day for maternal toxicity and 24.8 mg Co/kg/day for developmental toxicity.

Pregnant mice were dosed with 180 mg/kg/day (equivalent to 81.7 mg Co/kg/day) by oral intubation on days 8 through 12 of gestation. Mice were allowed to deliver, and neonates examined, counted, and weighed on the day of birth and postnatal day 3. Despite significant maternal weight reduction, there was no effect of cobalt on litter size, percent survival of neonates on postnatal days 1-3, or average neonatal weight. The NOAEL was determined to be 81.7 mg Co/kg/day under the conditions of this study.

When male rats were fed diet containing 265 ppm cobalt chloride hexahydrate (equivalent to 20 mg Co/kg at test initiation) for 98 days, degenerative and necrotic lesions in the seminiferous tubules were observed in animals. Cyanosis and engorgement of testicular vasculature on day 35 and thereafter was followed on day 70 by degenerative and necrotic changes in the germinal epithelium and Sertoli cells. Findings indicate that cobalt readily crosses the blood-testes barrier. Results of this study are highly consistent with others in which testicular degeneration and atrophy have been reported in rats exposed to 13.2 to 30.2 mg Co/kg/day as cobalt chloride for 2-3 months in the diet or drinking water.

After 12-13 weeks of exposure to 100, 200, or 400 ppm cobalt chloride hexahydrate (equivalent to 23.0, 42.0, or 72.1 mg Co/kg) in drinking water, male mice (5 per dose)

were evaluated for testicular weight, epididymal sperm concentration, sperm motility, sperm fertilizing ability, prostatic weight, seminal vesicle weight, and serum levels of testosterone. Cobalt exposure affected male reproductive parameters in a time- and dose-dependent manner. There was a significant decrease in testicular weight and epididymal sperm concentration after 11-13 weeks of exposure at all dose levels. Sperm motility and fertility were significantly depressed in the highest exposure groups. After cessation of exposure, some recovery was seen over time; however, indices remained significantly depressed through study termination.

Feeding diets containing 15% oleic acid to rats for 10-16 weeks had no adverse effects on the fertility of the male rats. Of 4 female weanling rats fed the diet, all 4 were able to become pregnant; however, 2 died at parturition, a litter was eaten at birth, and the remaining litter died within 3 days of birth. Mating of 7 adult female rats fed the diet for 10 weeks resulted in reproduction of 52 young, 44 of which survived 1 week and 11 of which survived 3 weeks. In all cases mammary development which normally occurs during pregnancy was markedly reduced, and lactation failed to occur. A few rats had ovarian cysts (Carroll and Noble, 1957).

Data were not identified for the evaluation of developmental and reproductive toxicity of cobalt oleate (CAS No. 14666-94-5). However, available data for the dissociation products allow use of scientific judgment to characterize the potential of cobalt oleate to cause developmental and reproductive toxicity. In addition, data from combined repeated dose with reproduction/developmental toxicity screening test (OECD 422) with the structural analog of cobalt oleate are under development by the Synthetic Organic Chemical Manufacturers Association Metal Carboxylates Coalition under the HPV program (see Table 2). Thus, no additional testing for genotoxicity is proposed.

Table 2. Mammalian Toxicity Data for Cobalt Oleate

ENDPOINT	Cobalt Oleate	Dissociation product Cobalt chloride	Dissociation product Oleic Acid
ACUTE			
Oral LD_{50} - Rat	9820 mg/kg (ra)	42.4 – 190 mg Co/kg	> 21.5 mL/kg
Dermal LD_{50} - Rabbit	NI	NI	>3000 mg/kg
Inhalation LC_{50} - Rat	NI	NI	NI
GENOTOXICITY			
Bacterial Reverse Mutation (Ames)	NI	Negative	Negative
Chromosome Aberration (Mouse micronucleus)	ra[1]	Positive	NI
REPEATED DOSE			
NOAEL - Rat	ra[1]	0.6 mg Co/kg/day (oral)	15% in diet (~7500 mg/kg/day)[2]
REPRODUCTIVE / DEVELOPMENTAL			
Developmental Toxicity NOAEL	ra[1]	24.8 mg Co/kg/day (rat) 81.7 mg Co/kg/day (mouse)	NI
Reproductive Toxicity	ra[1]	<13.2 mg Co/kg/day (rat) <23.0 mg Co/kg/day (mouse)	15% in diet (~7500 mg/kg/day)[2]

ra Based on read-across data from an analog substance, cobalt stearate
NI Data not identified
[1] Testing proposed for an analog substance by other HPV program
[2] Assuming the average feed consumption 20g/day by 400g rats

C. Aquatic Toxicity Data

Data for the dissociation products of cobalt oleate (cobalt and oleic acid), as well as for tall oil fatty acid are available to characterize potential environmental effects of cobalt oleate. The data employed are largely for the cobalt dissociation product and tall oil fatty acid and are summarized in Table 3. The work described in the HPV test plan prepared by the SOCMA Metal Carboxylates Coalition (2005) shows that cobalt chloride is similar to, or more bioavailable than the corresponding cobalt carboxylate salts, which makes cobalt chloride a conservative surrogate in estimating toxicity of dissociated cobalt.

Data were not identified for the effects of cobalt oleate to rainbow trout. Data are available for the dissociation product cobalt chloride, which exhibited a rainbow trout 96 h LC_{50} of 1.4 mg/L (Marr *et al.*, 1998). Data were not identified for oleic acid. However, data obtained from the Pine Chemicals Association, presented in a SOCMA HPV test

plan (2005) indicate that the 96 h *Pimephales promelas* (fathead minnow) LL_{50} for tall oil fatty acid, which contains oleic acid, is greater than 1000 mg/L, the highest loading rate tested.

Data were not identified for the effects of cobalt oleate on *Daphnia magna*. Cobalt chloride demonstrated a *Daphnia magna* 48 h EC_{50} of 1.52 mg Co/L (Khangarot *et al.*, 1987). Data were not identified for the effects of oleic acid on *Daphnia magna*. However, data obtained from the Pine Chemicals Association, presented in a SOCMA HPV test plan (2005) indicate that the 48 h *Daphnia magna* LL_{50} for tall oil fatty acid, which contains oleic acid is greater than 1000 mg/L, the highest loading rate tested.

Data were not identified for the effects of cobalt oleate on algae. Cobalt chloride demonstrated a 96 h algal (*Chlorella vulgaris*) EC_{50} of 0.52 mg/L (Rachlin and Grosso, 1993), while oleic acid demonstrated a nominal 96 h algal (*Selenastrum capricornutum*) IC_{50} of 0.58 mg/L (Kamaya *et al.*, 2003). However, this study employed a carrier solvent (DMSO), and the EC_{50} value appears to be greater than the aqueous solubility of oleic acid. Data obtained from the Pine Chemicals Association, presented in a SOCMA HPV test plan (2005) indicate that the 72 h *Selenastrum capricornutum* LL_{50} for tall oil fatty acid, which contains oleic acid, is 854.9 mg/L.

Although experimental data were not available to characterize the acute toxicity of cobalt oleate to fish, invertebrates and green algae, a quantitative structure-activity relationship to model cobalt oleate toxicity was applied. Modeling was performed using the ECOSAR computer model (Cash and Nabholz, 1990), a subroutine of the EPI Suite computer model. Results indicated that the compound may not be soluble enough to measure effects, and indeed, the neutral organic chemical class used by the model is likely inappropriate for a metal carboxylate such as cobalt oleate. This supports the use of data for the dissociation products as read-across data. ECOSAR results for oleic acid indicated that effects were unlikely to be seen at saturation. This is corroborated by the minimal effects observed in acute studies with tall oil fatty acid (Table 3), of which oleic acid is a major component.

Algal, *Daphnia magna,* and rainbow trout toxicity data for cobalt stearate, an analog of cobalt oleate, are under development by the SOCMA Metal Carboxylates Coalition under the HPV Program (Metal Carboxylates Coalition, 2005). These data will provide additional data to allow the use of scientific judgment to characterize potential environmental effects of cobalt oleate. Thus, no additional testing is proposed.

Table 3. Aquatic Toxicity Data for Cobalt Oleate

ENDPOINT	Cobalt oleate	Dissociation product Cobalt chloride	Tall oil fatty acid*
ACUTE			
Fish	NI[1]	1.4 mg Co/L (rainbow trout 96 h LC50)	>1000 mg/L (fathead minnow 96 h LL50)
Daphnia magna	NI[1]	1.52 mg/L (48 h EC50)	>1000 mg/L (48 h LL50)
Algae	NI[1]	0.52 mg/L (*Chlorella vulgaris* 96 h EC50)	854 mg/L (*Selenastrum capricornutum* 72 h EL50)

NI Data not identified
[1] Testing proposed for an analog (cobalt stearate) by the SOCMA Metal Carboxylates Coalition HPV test plan for cobalt stearate and fatty acids, tall oil, cobalt salts
* Data obtained from the Pine Chemicals Association through the SOCMA Metal Carboxylates Coalition HPV test plan for cobalt stearate and fatty acids, tall oil, cobalt salts

D. Environmental Fate Data

Biodegradation

Biodegradation of an organic substance by bacteria can provide energy and carbon for microbial growth. This process results in a structural change of an organic substance and can lead to the complete degradation of that substance, producing carbon dioxide and water.

Experimental data are not available to assess the biodegradability of cobalt oleate. The BIOWIN model, a subroutine within EPI Suite (2004) computer model estimates biodegradation of cobalt oleate to occur at a slow rate. However, the BIOWIN estimation for oleic acid predicts that it is readily biodegradable (EPISuite, 2004). The cobalt ion, as a metal, will not be degraded. Data from the Pine Chemicals Association in the SOCMA Metal Carboxylates Coalition HPV test plan (2005) show that both stearic acid, and tall oil fatty acids (which contain oleic acid) exhibit moderate to ready biodegradability (Metal Carboxylates Coalition, 2005). A biodegradation test for cobalt stearate is proposed in another HPV test plan. When available, these data can be considered read-across data for cobalt oleate. Thus, no additional testing is proposed.

Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (US EPA, 1999a) or estimated using an atmospheric oxidation potential (AOP) model accepted by the EPA (US EPA, 1999b). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation.

Cobalt oleate is not expected to volatilize to air based on a very low predicted vapor pressure. The dissociation product, oleic acid, which also has a very low vapor pressure, is predicted to very rapidly photodegrade, with a half-life of 1.7 h as calculated using the AOPWIN module of EPISuite (2004). This program calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a

standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.

Oleic acid has a calculated half-life in air of 1.7 hours, based on a rate constant of 75.5 x 10^{-12} cm^3/molecule*sec and an OH- concentration of 1.5 x 10^6 OH-/cm^3.

Stability in Water (Hydrolysis)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). The lack of a suitable leaving group renders a compound resistant to hydrolysis. Cobalt oleate is expected to be resistant to hydrolysis because it lacks a functional group that is hydrolytically reactive (Harris, 1982). Therefore, hydrolysis will not contribute to its removal from the environment.

Chemical Distribution in the Environment (Fugacity Modeling)

Fugacity-based multimedia modeling provides basic information on the relative distribution of a chemical between selected environmental compartments (i.e., air, soil, water, sediment, suspended sediment, and biota). A widely used fugacity model is the Level III model (Mackay, 1996) included in the EPI Suite program (2004).

The EPA guidance document (US EPA, 1999a) states that EPA accepts Level III fugacity data as an estimate of chemical distribution values. The input data required to run a Level III model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 4 compartments (air, soil, water, sediment) within a unit world. Level III data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical may to partition, based on selected physical parameters.

Results of the Mackay Level III environmental distribution model (Table 3) for cobalt oleate and a dissociation product, oleic acid suggest that these compounds will partition primarily to sediment and soil at similar levels. Despite differences in the input parameters, the distribution is similar, supporting the use of the calculated values for the HPV compound. Level III environmental distribution modeling by the SOCMA Metal Coalition (2005) resulted in virtually identical distributions for stearic acid, and tall oil fatty acid.

Table 4. Environmental Distribution as Calculated by the Mackay (2004) Level III Fugacity Model

Environmental Compartment	Cobalt Oleate Percent Distribution*	Oleic Acid**
Air	.01	.05
Water	1.89	3.86
Soil	28.4	28.2
Sediment	69.7	67.9

* Distribution is based on the following model input parameters for 9-octadedenoic acid (Z)-cobalt salt:

Molecular Weight	621.86	
Temperature	20°C	
Log K_{ow}	14.7	
Vapor Pressure	1.3×10^{-15} mm Hg	
Melting Point	313 °C	The melting point (MP) of the analog (cobalt stearate) is much lower than the calculated value for cobalt oleate. However, substituting the lower MP resulted in minimal change to the predicted distribution in the environment.

** Distribution is based on the following model input parameters for oleic acid:

Molecular Weight	282.47
Temperature	20°C
Log K_{ow}	7.64
Vapor Pressure	5.13×10^{-5} mm Hg
Melting Point	133 °C

IV. TEST PLAN SUMMARY

A search for existing studies/information on a structurally similar substance and dissociation products of cobalt oleate, and their review identified sufficient data and proposed testing under the existing HPV program to characterize all endpoints for cobalt oleate (Table 5).

A dossier containing the robust summaries of the data presented in this test plan is provided with this test plan. In addition, a test plan and robust summaries for the existing HPV category, Cobalt Stearate and Fatty Acids, Tall Oil, Cobalt Salts, is also provided.

Table 5. Data Characterizing Endpoints for Cobalt Oleate

Endpoint	Characterization / Value	Source
Physicochemical		
Melting Point (ºC)	313.2	EPI Suite, 2004
Boiling Point (ºC)	668.2	EPI Suite, 2004
Vapor Pressure (Pa @ 25ºC)	1.7×10^{-13}	EPI Suite, 2004
Water Solubility (mg/L@ 25ºC)	3.2×10^{-11}	EPI Suite, 2004
Log K_{ow} (25ºC)	14.71	EPI Suite, 2004
Environmental Fate		
Biodegradation	Slow (c)	EPI Suite, 2004
Photodegradation – Atmospheric oxidation (half- life; h)	1.7 (c)	EPI Suite, 2004
Hydrolysis	Hydrolysis will not contribute to degradation	Harris, 1982b Neely, 1985
Fugacity - Level III (Distribution to compartment)	Partitions primarily to: soil (28.4%); sediment (69.7%) (c)	Mackay *et al.*, 1996 EPI Suite, 2004
Aquatic Toxicity		
Freshwater Fish 96-hr LC_{50} (mg/L)	ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005
Freshwater Invert. 48-hr EC_{50} (mg/L)	ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005
Freshwater Alga 96-hr EC_{50} (mg/L)	ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005

Table 16 (continued). Data Characterizing Endpoints for Cobalt Oleate

Endpoint		Characterization / Value	Source
Mammalian Toxicity			
Acute	Inhalation	NI	
	Oral	Low toxicity LD_{50} = 9.8 g/kg bw (ra from cobalt stearate) (m)	Metal Carboxylates Coalition, 2005
	Dermal	Low toxicity LD_{50} = >3 g/kgbw (Oleic acid) (m)	CIR, 1987
Repeated Dose		ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005
Reproductive		ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005
Developmental		ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005
Geno-toxicity	Mutation	*S. typhimurium* Negative (ra from cobalt chloride, oleic acid) (m)	Metal Carboxylates Coalition, 2005 Mortelmans *et al.*, 1986
	Chromosome aberration (Mouse micronucleus)	ra from cobalt stearate (testing proposed by other HPV program)	Metal Carboxylates Coalition, 2005

m Measured for
c Calculated for
ra Read-across data from analog and/or metabolite as indicated
NI Data not identified

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APPENDIX A: RELIABILITY CRITERIA

Adapted from Klimisch *et al.* (1997)

Code of Reliability (CoR)	Category of Reliability
1	Reliable without restriction
1a	GLP guideline study (OECD, EC, EPA, FDA, etc...)
1b	Comparable to guideline study
1c	Test procedure in accordance with national standard methods (AFNOR, DIN, etc...)
1d	Test procedure in accordance with generally accepted scientific standards and described in sufficient detail
2	Reliable with restrictions
2a	Guideline study without detailed documentation
2b	Guideline study with acceptable restrictions
2c	Comparable to guideline study with acceptable restrictions
2d	Test procedure in accordance with national standard methods with acceptable restrictions
2e	Study well documented, meets generally accepted scientific principles, acceptable for assessment
2f	Accepted calculation method
2g	Data from handbook or collection of data
3	Not reliable
3a	Documentation insufficient for assessment
3b	Significant methodological deficiencies
3c	Unsuitable test system
4	Not assignable
4a	Abstract
4b	Secondary literature
4c	Original reference not yet available
4d	Original reference not translated (e.g. Russian)
4e	Documentation insufficient for assessment