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HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

ASSESSMENT PLAN

For The

LIGHT OXO FRACTIONS CATEGORY

CAS# 70955-03-2: Hexene, HOF, low-boiling
CAS# 68526-96-5: Heptene, HOF, low-boiling
CAS# 68938-03-4: Octene, HOF, low-boiling
CAS# 68526-93-2: Nonene, HOF, low-boiling
CAS# 68526-92-1: Dodecene, HOF, low-boiling

Submitted by:

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EXECUTIVE SUMMARY

Under the United States Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company has committed to voluntarily compile data for a category of substances defined as the Light Oxo Fractions. This category is supported by data for physicochemical, environmental fate and effects, and human health effects endpoints.

ExxonMobil Chemical Company considers the light oxo fractions (LOF) a category under the HPV Program because their physicochemical and toxicological properties are expected to be very similar and follow a regular pattern as a result of their chemical composition. Substances in this category are composed of olefins and paraffins. These substances are coproduct materials remaining from the production of alkyl alcohols via the hydroformylation of hexene, heptene, octene, nonene, and dodecene.

The hydroformylation process, involves the preparation of oxygenated organic compounds by the reaction of carbon monoxide and hydrogen (synthesis gas) with olefinic carbon compounds. Olefins which do not react, and paraffins produced by side reactions are the primary components of LOF.

The oxo reaction is performed under hydroformylation conditions in the presence of a carbonylation catalyst or catalyst precursor such as dicobaltoctacarbonyl, and results in the formation of a compound (e.g. an aldehyde) which has one more carbon atom in its molecular structure than the feedstock. Subsequent hydrogenation of the hydroformylation product leads to formation of the desired product alcohols. By virtue of the nature of the feedstock commonly available to industry, and indeed of the catalyst and reaction parameters employed, the hydroformylation reaction inevitably yields a range of products due to the numerous secondary reactions which take place.

Mixed LOF (REACH Registration Name: Alkenes, C6-10, hydroformylation products, low-boiling; no CAS RN) is a byproduct from C7-C11 alcohol production. Compositional analysis indicates Mixed LOF is approximately a 50/50% mixture of olefins and paraffins with a boiling point range of 102 – 182 °C. Based on composition and use it is appropriate to use data from Mixed LOF as read-across to the LOF Category CAS RNs.

Light Catalytic Cracked Naphtha (CAS RN 64741-55-5; LCCN) is a gasoline blending stream derived from refined petroleum. LCCN has a carbon range between C5-C10, a boiling point range from 37-168 °C, and consists of approximately 30% paraffins, 45% olefins, 10% naphthenics, and 13% aromatics. Based on composition and use, it is appropriate to use data from Light Catalytic Cracked Naphtha (CAS No. 64741-55-5) (LCCN) as read-across to the LOF Category CAS RNs.

The data for this group of substances will come from the Mixed LOF substance dossier that has been submitted under the EU REACH program, and the Gasoline Blending Streams Category Assessment Document submitted under the HPV Program.

The test data compiled for the category anchor studies is adequate to support a screening-level hazard assessment for the Light Oxo Fraction Category and its member substances (CAS numbers 70955-03-2, 68526-96-5, 68938-03-4, 68526-93-2, 68526-92-1). Member substances that lack measured data for selected HPV endpoints can be characterized by extrapolating or interpolating the existing data associated with the component chemicals. For some endpoints, computer modeled data can be used to further support a hazard assessment.

Evaluation of the light oxo fractions as a category has several advantages:

- The data from this category will be used to inform the public about the potential hazards of the light oxo fractions.
- Developing a data matrix of anchor studies and applying justifiable read across practices will provide a sufficiently robust data set to characterize each endpoint in the HPV Program without having to conduct a test for each endpoint and substance.
- This resourceful use of existing data will result in fewer animals needed for testing purposes while adequately assessing the potential hazards of substances in the Light Oxo Fraction Category.

Human Health

For human health endpoints, measured data on other complex substances that contain a similar range of chemical classes and carbon numbers were used. Read-across information indicates that these substances are not carcinogenic, mutagenic, or reproductive toxins.

Environment

For environmental endpoints, measured data on other complex substances that contain a similar range of chemical classes and carbon numbers were used. Read-across data for substances that represent the composition of the substances in this category show that these constituents can biodegrade to significant extents. Read-across data for substances that represent the composition of the substances in this category is available. A moderate level of acute toxicity in freshwater fish, invertebrates, and algae, is expected, based on LC50 and EC50 concentrations ranging from approximately 21 to 118 mg/L for read across substances.

Conclusions

The data available for mammalian and environmental endpoints on streams of similar complex hydrocarbon composition are sufficient to characterize the potential toxicity for substances in the Light Oxo Fraction Category.

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1 INTRODUCTION

Under the United States Environmental Protection Agency High Production Volume (HPV) Chemical Challenge Program (Program), ExxonMobil Chemical Company has committed to voluntarily compile data for a category of substances defined as light oxo fractions (LOF). This category is supported by data for physicochemical, environmental fate and effects, and human health effects endpoints.

ExxonMobil Chemical Company considers the light oxo fractions a category under the HPV Program because their physicochemical and toxicological properties are expected to be very similar and follow a regular pattern as a result of their chemical composition.

Substances in this category are composed of olefins and paraffins and are described as “alkyl alcohol overheads”. These substances are byproduct materials from the production of alkyl alcohols, which includes the hydroformylation of hexene, heptene, octene, nonene, and dodecene. Each contains a mixture of hydroformylation byproducts; approximately 50% olefins and 50% paraffins. Based on composition and use, it is appropriate to use existing data from Mixed LOF (REACH Registration Name: Alkenes, C6-10, hydroformylation products, low-boiling), and Light Catalytic Cracked Naphtha (CAS No. 64741-55-5) (LCCN) as read-across since both have similar composition and uses.

Evaluation of the Light Oxo Fractions as a category has several advantages:

- The data from this category will be used to inform the public about the potential hazards of the light oxo fractions.
- Developing a data matrix of anchor studies and applying justifiable read across practices will provide a sufficiently robust data set to characterize each endpoint in the HPV Chemical Challenge Program without having to conduct a test for each endpoint and substance.
- This resourceful use of existing data will result in fewer animals needed for testing purposes while adequately assessing the potential hazards of substances in the Light Oxo Fraction Category.

2 CHEMICAL PROCESS AND DESCRIPTION

The hydroformylation process, which in general terms is a process involving the preparation of oxygenated organic compounds by the reaction of carbon monoxide and hydrogen (synthesis gas) with carbon compounds containing olefinic unsaturation, and is particularly concerned with the treatment and recycling of byproducts of the primary oxo-reaction.

The oxo reaction is performed under hydroformylation conditions in the presence of a carbonylation catalyst or catalyst precursor such as dicobaltoctacarbonyl, and results in the formation of a compound e.g. an aldehyde which has one more carbon atom in its molecular structure than the feedstock. Subsequent hydrogenation of the primary product leads to higher alcohols. By virtue of the nature of the feedstock commonly available to industry, and indeed of the catalyst and reaction parameters employed, the hydroformylation reaction inevitably yields a range of products due to the numerous secondary reactions which take place.

3 CATEGORY JUSTIFICATION AND READ ACROSS RATIONALE

Substances in this category are composed of olefins and paraffins (approximately 50:50) and are described as “alkyl alcohol overheads”. These substances are byproduct materials from the production of alkyl alcohols, which includes the hydroformylation of hexene, heptene, octene, nonene, and dodecene. These streams each contain a mixture of hydroformylation reactants (olefins) and paraffins.

The olefin(s) and associated alcohol(s) by carbon number for the CAS numbers in this category are listed in Table 1. Exposure to Light Oxo Fractions is generally very low since these substances are recycled and used in feedstocks.

The members of this category each contain a mixture of hydroformylation reactants (olefins) and byproducts (paraffins). Thus, each member of the category is composed of the olefin and corresponding paraffin with an incremental change in carbon number for these components across the category.

The structural similarity of chemicals in each of the two groups creates a predictable pattern in the following parameters: physicochemical properties, environmental fate and effects, and human health effects. The compositional features of members of the category are as follows:

Table 1 - Light Oxo Fraction and their corresponding constituents: CAS Number and Carbon Number(s) of the Olefin and Paraffin for each of the LOFs.

CAS Number	CAS RN Name (common name)	Olefin	Paraffin
70955-03-2	Hexene, HOF, low-boiling (isoheptanol LOF)	C5-C6 (4%)	C5 (9%) C6 (66%) C7 (17%)
68526-96-5	Heptene, HOF, low-boiling (isooctanol LOF)	C7 (33%)	C7 (66%)
68938-03-4	Octene, HOF, low-boiling (isononanol LOF)	C8 (57%)	C8 (41%)
68526-93-2	Nonene, HOF, low-boiling (isodecanol LOF)	C9 (57%*)	C9 (41%*)
68526-92-1	Dodecene, HOF, low-boiling (isotridecanol LOF)	C12 (57%*)	C12 (41%*)
N/A	Mixed LOF**	C7-10 (50%)	C7-10 (50%)
64741-55-5	LCCN**	C5-10 (45%)	C5-10 (30%)

* Read Across from CAS RN 68938-03-4

** Existing data available for read across to the five LOF CAS RNs

N/A Not Available

Evaluation of the light oxo fractions as a category accomplishes the goal of the Challenge Program - to obtain screening level hazard information - through the strategic evaluation of data for substances within this category. The test plan strategy is based on the principle that:

These substances behave in a similar and/or predictable manner, and interpolation and extrapolation of data can be used to characterize the light oxo fractions for which data are not available.

Procedures to assess the reliability of selected studies described in this test plan are based on the guidelines described by Klimisch *et al.*, 1997.

4 PHYSICAL-CHEMICAL PROPERTIES

Physicochemical data (i.e. melting point, boiling point, vapor pressure, water solubility, and Kow) for selected chemical components in the Light Oxo Fraction Category were not available. Read-across data for substances that represent the composition of the substances in this category were used to fulfill the HPV endpoints. These data are presented as ranges.

Table 2 lists selected measured physicochemical data (boiling range, vapor pressure) as they appear in attached robust summary documents. These data are provided with this test plan to further justify these substances as a distinct category under the HPV Program.

Table 2 - Selected Physical Properties of Light Oxo Fraction Substances

CAS NUMBER	CHEMICAL NAME	PRIMARY COMPONENTS	BOILING RANGE (° C)	VAPOR PRESSURE	WATER SOLUBILITY (mg/L)**	LOG Kow
N/A	Mixed LOF (RA)	C7-10 olefins and paraffins (50:50)	102-182**	<2.9 psi (50°C)	N/A	N/A
64741-55-5	LCCN (RA)	C5-C10; 30% paraffins, 45% olefins, 10% naphthenics, and 13% aromatics	37-168	10.3 psia	4.6	2.13-4*

N/A not available

RA Read Across

* Calculated using EPIWIN (see robust summary attached; EPA, 2008)

** Measured values (EM Mixed LOF REACH IUCLID Dossier, 2010)

5 ENVIRONMENTAL FATE

5.1 Environmental Fate Endpoints

5.1.1 Biodegradation

Upon review of the available information, sufficient data were identified to accurately characterize the biodegradability of the substances in this category (Table 3). The LOF Category is expected exhibit biodegradation (28 days) of approximately 52%. These read across data were developed for Mixed LOF, using a non-acclimated inocula obtained from wastewater treatment plants. The tests used closed systems which are recommended when assessing the biodegradability of materials with a potential to volatilize, like those in this category. The test systems were continuously stirred, which is also recommended when evaluating mixtures containing several chemicals, some of which may have minimal water-solubility. A second study using an adapted innoculum (EPA, 2008) resulted in 74.3%

biodegradation after 28 days, and provides further evidence for the inherent biodegradability of the substances in the LOF Category.

Table 3 - Light Oxo Fraction Data Matrix for Biodegradation

CAS #	Substance Name	Percent Biodegradation 28-days*
N/A	Mixed LOF	52% (RA)
64741-55-5	LCCN	74.3%** (RA)

* Measured data

** Adapted inoculum

RA Read Across

5.1.2 Photodegradation

5.1.2.1 Photodegradation – Photolysis (Direct)

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (1977).

In general, most representatives of the LOF category do not contain component molecules that will undergo direct photolysis. Saturated hydrocarbons (paraffins) and olefins with one double bond, which constitute the majority of these components, do not absorb appreciable light energy above 290 nm. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

5.1.2.2 Photodegradation – Atmospheric Oxidation (Indirect)

Photodegradation can be measured (US EPA, 1999a) or estimated using models accepted by the EPA (US EPA, 1999b). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Chemicals, such as those in the Light Oxo Fraction Category, have the potential to volatilize to air.

In air, chemicals can undergo reaction with photosensitized oxygen in the form of hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hour day, and a given OH- concentration. This calculation was completed for representative components of LCCN (EPA, 2008).

AOPWIN ver. 1.89 calculates atmospheric oxidation half-lives of hydrocarbons in contact with hydroxyl radicals in the troposphere, under the influence of sunlight and in contact with O³. Atmospheric oxidation rates were calculated for the C5 to C9 hydrocarbon components found in LCCN CAS No. 64741-55-5. Detailed hydrocarbon analysis performed by Chevron Research was used to identify the components of this specific LCCN sample. Based on a 12-hour day, the range for atmospheric half-lives for LCCN constituents due to OH reactions is: 1.44 hours to 15.98 days. The range for atmospheric half-lives due to O³ reactions for LCCN olefinic constituents (accounting for approximately 30% composition) is 38.38 min to 22.92 h.

5.1.3 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).

Stability in water can be measured (US EPA, 1999a) or estimated using models accepted by the EPA (US EPA, 1999b). However, the substances included in the LOF Category are mixtures of olefins and paraffins and do not contain chemical bonds/groups that will hydrolyze. As such they are not expected to hydrolyze at a measurable rate.

5.1.4 Chemical Transport and Distribution

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay, 1996). EPA cites the use of this model in its document titled Determining the Adequacy of Existing Data (US EPA, 1999a), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Results of Level I models are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition in the environment. One drawback of these and higher level models is their inability to predict the distribution of the entire set of constituents comprising complex petroleum streams. To gain an understanding of the potential environmental distribution for these complex substances, modeling was performed for individual

hydrocarbon compounds that had been identified through detailed hydrocarbon analyses to exist in these streams. The hydrocarbons selected for modeling were not only those identified to exist in these substances, but also spanned a wide range of molecular weights and hydrocarbon types. The resulting values represent the potential ranges of distribution to environmental media for those hydrocarbon constituents found in these streams. These data were used as read across to the substances in the Light Oxo Fraction Category.

Air:	97-100%
Water:	0.01-2.7%
Soil:	≤1.2%
Sediment:	≤0.001 - 0.02%
Suspended sediment:	≤0.001 – 0.02%

Conclusion: Fugacity modeling for those constituents in LCCN indicates that, at steady state, these components partition ≥97% to air, while partitioning into soil or water does not exceed 1.2% or 2.7%, respectively. Partitioning to sediment or suspended sediment is minimal.

6 ENVIRONMENTAL EFFECTS

6.1 Aquatic Toxicity

Aquatic endpoints for the HPV Program include acute toxicity to a freshwater fish and invertebrates, and alga. Read across data were identified to adequately characterize the aquatic toxicity of the substances in the Light Oxo Fraction Category.

Table 4 identifies the type of data available for the components of each substance and the read across strategy applied to the data gaps. Table 4 summarizes the available data used to characterize the aquatic toxicity of LOF substances.

Table 4 - Light Oxo Fraction Data Matrix for Aquatic Toxicity

CAS #	Substance Name	Fish Acute Toxicity	Invertebrate Acute Toxicity	Algal Toxicity
N/A	Mixed LOF (RA)	96 h LL50: 21 mg/L ^a	N/A	N/A
64741-55-5	LCCN (RA)	96 h LL50: 46 mg/L ^b	48 h EL50: 18 mg/L ^b	96 h EL50: 64 mg/L ^b

RA-read across

N/A-not available

a data from Mixed LOF REACH IUCLID Dossier

b data from Gasoline Blending Streams Category Assessment Document (USEPA, 2008)

6.1.1 Fish Acute Toxicity

Acute experimental toxicity test results are reported for rainbow trout (*Oncorhynchus mykiss*) for Mixed LOF, and fathead minnow (*Pimephales promelas*) for LCCN (Table 4). These data show that there is potential for acute toxicity, with LL50s of 21 and 46 mg/L, respectively. The carbon number range of olefins and paraffins in Mixed LOF and LCCN are similar to those in the substances in the

LOF Category, which can be expected to demonstrate similar toxicity. Thus data for these two substances are appropriate for evaluating the LOF Category.

6.1.2 Invertebrate Acute Toxicity

An acute experimental toxicity test result is reported for a daphnid (*Daphnia magna*) for LCCN (Table 4). This data shows that there is potential for acute toxicity, with an LL50 18 mg/L. The carbon number range of olefins and paraffins in LCCN is similar to those in the series of substances in the LOF Category, which can be expected to demonstrate similar toxicity. Thus data for LCCN is appropriate for evaluating the LOF Category.

6.1.3 Algal Toxicity

An acute experimental toxicity test result is reported for the freshwater alga (*Selenastrum capricornutum*) for LCCN (Table 4). This data shows that there is potential for acute toxicity, with an LL50 of 64 mg/L. The carbon number range of olefins and paraffins in LCCN is similar to those in the series of substances in the LOF Category, which can be expected to demonstrate similar toxicity. Thus data for this substance is appropriate for evaluating the LOF Category.

7 HUMAN HEALTH EFFECTS

7.1 Human Health Effects

The body handles aliphatic hydrocarbons in a similar manner via oxidative conversion to alcohols, ketones, and eventual elimination as carbon dioxide and carboxylic acids (Wislocki *et al*, 1980). The un-degraded alcohols can be conjugated either directly or as a metabolite with glucuronic acid, sulfuric acid, or glycine and are rapidly excreted (Lington and Bevan, 1994). Intermediate aldehydes could be reactive and bind with DNA and/or proteins. Glucuronidation and glutathione conjugation are possible means of rapid elimination (Mann, 1987).

Table 5 summarizes the available data used to characterize the toxicity of the light oxo fraction category.

Table 5 - Light Oxo Fraction Summary Toxicology Data

CAS #	Substance name	Acute Toxicity	Genotox. Point Mutation	Genotox. Chrom. Aberr.	Subchronic Toxicity NOAEL	Developmental Toxicity NOAEL
N/A	Mixed LOF	N/A	N/A	N/A	N/A	N/A
64741-55-5	LCCN	>5 g/kg/day	Negative	Negative	Rat systemic NOAEC 2136 ppm Rat systemic dermal NOAEL > 3g/kg	Rat inhalation NOAEC Reproductive/Developmental parameters 7500 ppm

7.1.1 Acute Toxicity

Light catalytic cracked naphtha (API 83-20; CAS #64741-55-5, approx. 46% olefinic) is not acutely toxic by the oral (rat > 5000mg/kg), dermal (rabbit > 3000mg/kg) and inhalation (rat > 5.3mg/l, 4 hr exposure) routes and is not irritating to the rabbit eye 24 hrs after exposure. It is a moderate skin irritant in rabbits but is not a skin sensitizer in guinea pigs. (API, 1986a, 1987a)

7.1.2 Repeated Dose Toxicity

Light catalytic cracked naphtha (LCCN, CAS #64741-55-5, approximately 46% olefinic) was tested by inhalation in three 13-week studies and one 21-day study. In the three 13 week studies, concentrations were 147 - 2136ppm (530-7690 mg/m³) partially vaporized LCCN to rats and mice (Dalbey *et al.*, 1996a,b); 1500 – 4500ppm (5474-16423 mg/m³) wholly vaporized LCCN to rats (API, 1987d); and 750 – 7500ppm (2336-23364 mg/m³) light ends distillate to rats (Lapin *et al.*, 2001). In the 21-day study (15 actual exposures), wholly vaporized LCCN was administered to male and female Sprague Dawley rats at concentrations of 55, 567, and 3628ppm (200, 2040, and 13060mg/m³) (Halder *et al.*, 1984).

Sprague Dawley rats [16 males/16 females/group] were exposed to an LCCN light end distillate (approx. 60% olefinic) at concentrations of 0, 750, 2500, and 7500ppm (2340, 7700 and 23400mg/m³), 6 hours/day, 5 days/wk over 15 weeks, according to OECD guideline 413, for a total duration of at least 65 exposures. The test material (LCCN-D) was prepared to be representative of the fraction of light catalytic cracked naphtha to which man might be exposed during normal handling and blending. The maximum exposure level was 75% of the lower explosive limit for LCCN distillate. Extra groups of 16 rats of each sex exposed to the high dose level and a recovery control group were maintained untreated for 28 days following cessation of the 15 weeks exposure. Neurobehavioral evaluations of motor activity and functional activity [FOB] were performed pretest and during weeks 5, 9, 15 and 19 for recovery groups. Animals were not exposed to LCCN-D during these tests. Ophthalmoscopic evaluations were performed pretest and just prior to the scheduled sacrifices at 15 weeks and 20 weeks (recovery groups). Body weights and food consumption was measured throughout the study. Blood samples were taken from 10 fasted rats/sex/group at 14 and 18 weeks for hematological and clinical chemistry measurements. At termination (after 15 weeks exposure for the main study and after 19 weeks for the recovery animals) all animals were killed and subjected to a complete macroscopic examination. Ten rats/sex/group were selected for non-neuropathologic examination and 6 rats/sex/group for neuropathologic examination. The following organs were weighed from the non-neuropathologic animals: adrenals, brain, heart, kidneys, liver, lung, ovaries, prostate, spleen, testes (with epididymides), thymus and uterus. Brain lengths and widths were measured for each rat. Thirty-nine tissues removed from the control and high dose animals, fixed and examined histopathologically. Additionally, kidneys from selected animals were stained with Mallory-Heidenhain and examined. Tissues were collected from the nervous system (central and peripheral) of all animals and nervous system tissues were selected randomly from 6 rats per sex/group in the high dose and controls at the end of 15 weeks for microscopic examination. Specific brain regions examined were forebrain, cerebral cortex, hippocampus, basal ganglia, midbrain cerebellum and pons and medulla.

Neurobehavioral studies included motor activity, monitored as the number of beam breaks in an activity box, at pretest, and during weeks 5, 9, 14, and at the end of the 4 week recovery period. The Functional Operational Battery [FOB] was comprised of home cage evaluations, handling and open field behaviors and reflex assessment. Animals were also evaluated for fore limb and hind limb grip strength, landing foot splay and air righting ability.

No exposure-related clinical observations were noted either during exposure or during non-exposure periods and no ocular abnormalities were observed. Slight differences in weight gain were seen in high dose animals but weights were comparable to controls at the end of the recovery period. During the 4-week recovery period, the high dose males and females had food consumption that was greater (statistically significant) than controls. At 15 weeks, hematologic changes in the high dose group were decreased hemoglobin (8%) and hematocrit (7%) in males and decreased MCHC (3%) in females and in the mid-dose group males decreased MCHC (4%). After 4 weeks recovery, all hematologic values were comparable to controls. No abnormal clinical chemistry values were observed after 15 weeks exposure. Although glucose and albumin levels were elevated in high dose females after the recovery period, the values fell within normal historical range and were not considered toxicologically significant. Statistically significant increases in absolute and relative kidney weights in high dose males and relative kidney weights in mid-dose males correlated with microscopically observed hyaline droplet formation and degeneration of proximal renal tubules in high dose males, indicative of alpha 2-microglobulin mediated nephropathy, also identified as light hydrocarbon nephropathy, a species and sex specific syndrome not relevant to humans (US EPA, 1991). Increased relative liver weights in high dose rats of both sexes had no microscopic correlate, although the absolute liver weight in recovery high dose females was elevated possibly correlated with increased food consumption. Decreased relative brain weight in recovery females had no microscopic correlate. With the exception of kidney findings in males, the only treatment related microscopic observations were nasal mucosa hyperplasia and hypertrophy/ hyperplasia of goblet cells indicative of exposure to a mild irritant, the incidence of which was comparable to controls after the recovery period.

In the neurobehavioral studies there was no evidence of any effect on motor activity either after 15 weeks exposure or after the 4-week recovery period. There was no evidence of a treatment-related effect in the functional operational battery. The systemic toxicity LOAEL = 7500ppm (23400mg/m³) based on increased organ weight and nasal epithelium changes and the NOAEL = 2500ppm (7700mg/m³). The Neurotoxicity NOAEL = 7500ppm (23400mg/m³). (Lapin *et al.*, 2001)

A 13 week inhalation study was conducted in Sprague Dawley rats [10/sex/group] and CD-1 mice [10/sex/group] exposed to a 40% vapor of LCCN at concentrations of 0, 147, 572, 2136ppm (0, 530, 2060 & 7690 mg/m³), 6 hours/day, 5 days/week. Extra groups of 10 rats and mice of each sex served as sham and untreated controls. Food and water was available ad-lib, except during the exposure periods. Clinical observations were made regularly and body weights were recorded weekly. At the end of the 13 weeks exposure, blood was drawn from fasted animals for hematological and clinical chemistry measurements. All animals were then sacrificed and necropsied. Organs were weighed and a wide range of tissues fixed for subsequent histology and microscopic examination. The wet and dry weights of the right apical and right middle lung lobes were also recorded. The cauda epididymis of the control and high dose male rats was used to determine the morphology and number of sperm and the left testis was used to determine the number of testicular spermatids. The following tissues from the high dose and sham treated animals were examined histologically: adrenals, kidney, bone and marrow (sternum), pancreas, brain, submaxillary salivary gland, eye, optic nerve, spleen, heart, stomach, colon, testes or ovaries, duodenum, kidneys, thymus, thyroid, liver, tracheobronchial lymph nodes, lung (left lobe), nasal turbinates, muscle, urinary bladder, sciatic nerve, and any gross lesions. Additional sections included lung from untreated controls and kidney from 0, 572 and 2136ppm (2060 and 7690 mg/m³) exposure groups.

No treatment-related changes were observed in either species in clinical signs, body weight, clinical chemistry or hematology except four male rats in the high dose group that had lesions on the skin in the scrotal area. This was attributed possibly to an interaction between abrasions of the skin against the floors of the cages and the whole-body exposure to high concentrations of LCCN. Organ weights were unaffected in either species, except for uterus weights. Uterine weights in the rats were less than untreated controls for all exposed groups, but not less than the sham controls. Uterine weight changes were not considered to be related to LCCN because they were not dose-related, and there was no difference between the sham and untreated controls. Additionally, no similar effect was observed in the mice. No treatment-related abnormalities were observed in any of the organs examined microscopically. The occurrence of hyaline droplets in dilated renal tubules was similar in the controls and the high dose male rats. The number of sperm per gram of cauda epididymis was significantly lower in the 2136ppm (7690 mg/m³) rat group than in the sham controls but not the untreated controls. The actual number of epididymal sperm was not significantly affected by exposure. Also, the number of testicular spermatids and the percentage of abnormal sperm in the cauda epididymis were not affected by exposure to 2136ppm (7690 mg/m³) in rats compared to either control group. The toxicological significance of the decrease in sperm/gram in the epididymis is unknown since it was not supported by other male parameters, but the occurrence has been used to set the LOAEL. The rat systemic toxicity LOAEL = 2136ppm (7690 mg/m³) NOAEL = 572ppm (2060 mg/m³). The mouse systemic NOAEL = 2136ppm (7690 mg/m³). (Dalbey *et al*, 1996a,b)

Another 13 week inhalation study on a high olefinic test material similar to those used in the Dalbey *et al* (1996a,b) and Lapin *et al* (2001) studies conducted in rats at exposure concentrations of 1510, 2610, 4520 ppm (0, 5475, 9500, -16425 mg/m³) had results similar to the Lapin *et al* study. Additionally, a trace centrilobular hepatocellular hypertrophy was observed in 50% of the males and 25% of the females in the 4520 ppm group. This study was performed at vapor concentrations above that of the 40% vapor study of Dalbey *et al* (1996 a,b), and did not show any effects on sperm numbers in the epididymis. (API 1987d).

The 21 day inhalation study set of Halder *et al*, 1984 confirmed the findings in male kidneys that had been observed in other studies with rats. However, since these kidney effects are not considered relevant to man and study duration is less than the 13 week studies, this is not considered a key study and is not included in establishing toxicity ranges.

Light catalytic cracked naphtha (LCCN, CAS #64741-55-5, approximately 46% olefinic) was tested for 13 weeks in Sprague Dawley rats. LCCN was applied undiluted to the clipped backs of rats (15/sex/group) at concentrations of 0, 30, 125 or 3000mg/kg/day, 5 days/week for 90 days. Rats were fitted with Elizabethan collars to minimize ingestion of test material. Percutaneous absorption was assessed by applying LCCN containing radiolabeled n- octane in a non-occlusive Bronaugh cell to untreated animals and animals treated for 90 days with cold LCCN. The percent of applied dose was recovered in urine, feces and tissue over 96 hours. No systemic toxicity expressed as changes in body or organ weights, clinical observations, hematology or clinical chemistry parameters, gross pathology or histopathology with the exception of skin irritation at treated sites resulted from exposure to LCCN. Sperm morphology in treated rats was comparable to controls. Skin irritation, erythema and edema at treated sites and histopathologic correlates of hyperplasia, inflammation and ulceration in all groups in a dose related pattern were the only effects reported. Approximately 1% radiolabeled LCCN penetrated the skin over 96 hours. Bioavailability was similar for untreated rats and those pre-treated for 90 days with LCCN. (Mobil 1988)

7.1.3 Genetic toxicity

7.1.3.1 Genetic toxicity – *In Vitro*

Three samples of light catalytic cracked naphtha (LCCN, approx. 46% olefinic) have been tested in a mouse lymphoma (L5178Y TK+/-) forward mutation assay. The results for API 83-20 are described here (API, 1987b). A cytotoxicity study carried out prior to the mutagenicity assay established that LCCN was highly toxic at 500nl/ml without activation and lethal at the same concentration in the presence of metabolic activation. For the initial mutation assay the mouse lymphoma cells were exposed for 4 hours to LCCN at treatments from 50 to 800 nl/ml LCCN without activation and with treatments from 25 to 500 nl/ml LCCN with Aroclor-induced rat liver S-9 activation. After exposure to LCCN, the cells were allowed to recover for 2 days and then cultures were selected for cloning and mutant selection. Plates containing colonies of selected cells were incubated for 10 to 14 days after which they were scored for total number of colonies per plate. A mutation frequency was then determined. Due to a wide range of toxicity in the first assay with and without metabolic activation, a second assay was performed over a narrower dose range of 50 to 150nl LCCN without S9 activation and 200 to 300nl LCCN with activation. LCCN sample API 83-20 was not mutagenic with or without metabolic activation. Of the two other LCCN samples tested, one API 81-03 (API, 1985a) was not mutagenic and one API 81-04 (API, 1986b) was not mutagenic without metabolic activation but gave equivocal results with metabolic activation. Equivocal results are defined as a situation in which one or more doses exhibit a 2-fold mutant frequency greater than background level but there is no dose response. Overall LCCN is not considered mutagenic in this mammalian cell assay.

An *in vitro* sister chromatid exchange (SCE) assay in Chinese hamster ovary (CHO) cells with and without metabolic activation [a non-SIDs endpoint] was performed with LCCN. CHO cells were seeded in duplicate for each treatment condition and were incubated at 37°C in a humidified atmosphere for 16 to 24 hours. Treatment was carried out by re-feeding two complete sets of flasks with complete medium for the non activation study or with Aroclor-induced rat liver S-9 reaction mixture for the activated study to which was added 50 µl of dosing solution of test control or article in solvent or solvent alone. CHO cells were exposed to solvent alone and to nine concentrations of LCCN ranging from 1 to 0.0001µl/ml in the absence and presence of an S-9 reaction mixture. Based on the growth inhibition and cell cycle delay, dose levels of 0.3, 0.2, 0.1 and 0.05 µl/ml LCCN were selected for use in the assay without metabolic activation and at concentrations of 0.2, 0.1, 0.05 and 0.03 µl/ml LCCN in the assay with metabolic activation. A harvest time of 30 hours after treatment initiation was selected to assure collection of enough analyzable second division metaphases at the high dose. In the non-activation study the cells were exposed for 28 hours. Two hours after exposure 0.01 mM BrdU was added to the treatment medium. At the end of the treatment period, the treatment medium was removed, the cells were rinsed and were then exposed to colcemid (0.1µg/ml) for a further 2 hours. In the activation study exposure was for 2 hours. After the exposure period, the treatment medium was removed; the cells were washed with PBS, re-fed with medium containing BrdU and then incubated for a further 28 hours. Colcemid was added at a final concentration of 0.1µg/ml for the last 2 hours of incubation. For activated and non-activated assays, metaphase cells were harvested 2 hours after addition of colcemid. Cells were collected and fixed and stored until slides were prepared. Slides were coded and scored without regard to treatment group. Only cells with $20 \leq 2$ centromeres were selected for evaluation of SCEs. A total of 4 doses were scored including the highest test article dose where sufficient second-division metaphase cells were available. SCEs were scored in 25 cells from each duplicate culture to make up a total of 50 cells per treatment. The percentage of cells in first (M1), second (M2) or third division (M3) metaphase was also recorded for a total of 100 metaphase cells scored. Triethylenemelamine (TEM) was used as positive control at a concentration of 0.025 µg/ml. in

the non-activated assay. In the activated assay cyclophosphamide (CP) was used at a concentration of 2.5µg/ml. API 81-03 did not induce an increase in sister chromatid exchanges in CHO cells when tested in the absence of metabolic activation. However the test material did induce a small but statistically significant increase in SCEs at two intermediate dose levels in the presence of metabolic activation, a result that was concluded to be equivocal. (API 1988a)

7.1.3.2 Genetic toxicity – *In Vivo*

Samples of light catalytic cracked naphtha (approx. 46% olefinic) were tested in two rat chromosome assays [intraperitoneal and inhalation] and in an in vivo mouse sister chromatid exchange (SCE) assay. LCCN (API 81-04) was tested in a Sprague Dawley rat chromosome aberration assay [15/sex/group] at doses of 0.3, 1.0, and 3.0g/kg in corn oil, administered intraperitoneally in a single dose. Two to four hours prior to sacrifice the rats were given a single intraperitoneal dose of colchicine (1 mg/kg). Animals [5/sex/group/time] were sacrificed at 6, 24 and 48 hrs post dose. A group of 5 animals of each sex to be used as positive controls was dosed with triethylenemelamine (TEM) at a level of 0.5 mg/kg and these animals were killed at 24 hours postdose. Bone marrow was harvested from the femurs of treated rats, processed and stained for cytogenetic examination [a minimum of 50 metaphase spreads per animal]. There was a 9% weight loss in males 48 hours after receiving 3 g/kg API 81-04 and a 2% weight loss in females at the same time and dose level. Clinical signs of toxicity in the 3g/kg group included lethargy in both sexes and increased tearing as indicated by a crusty appearance of fur around the eyes of the male animals. No chromosome aberrations, rearrangements, or cell cycle disruption were observed in any dose group (API, 1985b).

In a separate study in which exposure was by inhalation at 63, 297 and 2046 ppm, 6hr/day for 5 days, there was no evidence that light catalytic cracked naphtha (API 81-03) caused chromosomal aberrations in rats. (API, 1985a)

LCCN (API 81-03) was tested in a mouse [B6C3F1; 5/sex/group] sister chromatid exchange (SCE) assay [a non-SIDS endpoint] at doses of 0.2, 1.2, and 2.4 g/kg in corn oil, administered intraperitoneally in a single dose. Four hours prior to administration of test material, the mice were anesthetized with Metofane and an agar-coated 50mg BrdU pellet was implanted subcutaneously in the lower abdominal region. The positive control (cyclophosphamide) was injected ip at a dose level of 10 mg/kg. A second positive control (API 81-15, catalytic cracked clarified oil) was administered at a dose of 4 g/kg, which was administered by ip injection at a rate of 10 ml/kg. Colchicine, used to arrest dividing cells in metaphase, was administered ip at 1 mg/kg to all mice two to four hours prior to sacrifice. 24 to 26 hours after BrdU pellet implantation the mice were sacrificed. Marrow was collected from both femurs. After washing and fixing bone marrow cells slides were prepared for subsequent staining and examination. Two to five slides were prepared from each animal. A minimum of 50 second-division metaphase spreads from each animal were examined and scored for SCEs and chromosome number. The mitotic index was recorded as the percentage number of cells in mitosis based upon 500 cells counted. The percentage of first, second and third-division metaphase cells was also recorded as the number per 100 cells counted. There was a significant increase in SCEs/cell when analyzed by sex. Pairwise comparisons by sex of each treatment group with its vehicle control were significantly different. (API, 1988c)

Although the SCE assay demonstrated interaction of LCCN and DNA, it was not considered definitive for clastogenic activity since no genetic material was unbalanced or lost. SCE can be regarded as more a biomarker of exposure rather than as indicator of mutagenic effect. Negative results in two assays,

which visualize actual cytogenetic damage demonstrate that LCCN is not a clastogenic material (API, 1985b,c)

7.1.4 Reproductive and Developmental Toxicity

Light catalytic cracked naphtha (CAS #64741-55-5, LCCN, approx. 42% olefinic) was tested in rats in an OECD 421 Inhalation Reproductive and Developmental Toxicity Screening Test as a light end distillate (approx. 60% olefinic). Male and female Sprague Dawley rats (10/sex/group) were exposed to concentrations of 0, 750, 2500 and 7500ppm (2700, 9000 and 27000mg/m³), 6 hours/day, 7 days/week for 2 weeks prior to mating. The maximum exposure level was 75% of the lower explosive limit for LCCN distillate. Parental males and females who failed to mate were exposed during mating and 23 additional days following completion of the mating period. These animals were sacrificed shortly after the last litters were delivered reached post partum day 4. During the mating period, females were exposed until evidence of mating was observed. If there was no evidence that mating had occurred the pairs were allowed to remain together up to a period of 2 weeks. Pregnant females were treated daily during gestation (GD days 0-19) until sacrificed on post-natal day 4. Viability, clinical observations, body weights, feed consumption, and survival were evaluated in parental rats. At necropsy each parental animal was examined macroscopically for structural abnormalities and pathological changes with emphasis on reproductive organs. The following organs were weighed and organ/body weight ratios were calculated: adrenals, brain, heart, kidneys, liver, lung, spleen, epididymides, testes and thymus. Twenty-seven tissues were preserved from all adult animals in all dose groups. Ovaries, testes, epididymides, nose with nasal turbinates, and any grossly observed abnormalities were processed and sections examined histologically for all males and female parental animals in the control and highest dose group. Reproductive parameters (mating indices, pregnancy rates, male fertility indices, gestation length, number of implantation sites and corpora lutea, pre- and post-implantation loss, pups per litter, live born and stillborn pups, and incidence of dams with no viable pups) and developmental endpoints (pup physical examination, viability, weight, sex ratio, litter survival indices and mean pup survival indices) were evaluated. Pups were sacrificed on day 4 of lactation and underwent a complete macroscopic examination and a determination of sex by internal examination. All pups were preserved with viscera intact. Pups found dead at birth and that died prior to day 4 of lactation also underwent a gross external and internal examination. Dead pups were not eviscerated, but were preserved intact.

All groups had a fertility index of >90% and a live birth index greater than or equal to 98%. Offspring showed comparable body weights, weight gain, and viability index at postnatal day 4. Parental male rats had increased kidney weights and relative liver weights at the highest dose, and high dose females had increased spleen weights. Reproductive organs and nasal turbinates from high dose and control animals were examined by a pathologist and no histological changes were observed in tissue from treated rats. LOAEL parental toxicity = 7500ppm [27000mg/m³] NOAEL parental toxicity = 2500ppm [9000mg/m³]; NOAEL reproductive performance/ developmental toxicity = 7500ppm [27000mg/m³] (Schreiner *et al.*, 1999).

An Inhalation Developmental toxicity screening study in Sprague Dawley rats [10/sex/group] and CD-1 mice [15 presumed pregnant females/group] exposed to a 40% vapor of LCCN at concentrations of 0 [untreated controls], 0 [sham-treated controls], 597, 2128ppm [2150 & 7660 mg/m³], 6 hours/day, for gestation days 0-19. The vapor contained approximately 41% olefins. All animals were observed daily and body weights were recorded on days 0, 6, 13 and 20 of gestation. On day 20 each female was sacrificed and all organs were examined grossly. Serum samples were analyzed for a variety of parameters, including serum iron and lactic dehydrogenase. The number of corpora lutea per ovary and

the gravid uterine weights were recorded. Uterine contents were examined and the numbers of implantation sites, early resorptions and live and dead fetuses recorded. Each fetus was identified for its sex, was weighed and the crown-rump distance was measured. Each fetus was examined for external anomalies. Half the fetuses were fixed in Bouin's solution and examined for visceral anomalies and the remaining fetuses were prepared for examination for skeletal anomalies.

There were no treatment related clinical abnormalities or differences in body weights among dams or adverse effects on reproductive parameters with the exception of a statistically significant increase in resorptions and percent resorptions at the 2128ppm dose [10.4% vs 4.6% in untreated controls and 3.9% in sham controls] and an increased incidence of high dose dams with resorptions compared to sham but not to untreated controls. The authors considered the biological significance of the increase in resorptions to be uncertain because the number of viable fetuses (i.e. litter size) in this group were comparable to litter size in other groups and the mean incidence of resorptions in the control groups from previous studies at this facility ranged from 3.0 to 11.2% compared to the 10.4% in the 2128ppm group. No visceral abnormalities were observed. There were an increased number of skeletal variations in animals housed in the exposure chambers (exposed and sham treated controls) when compared to the untreated controls. The authors concluded that these alterations were not related to LCCN since they occurred at a similar incidence in the sham treated controls as well. Despite the reservations of the authors, the developmental LOAEL is identified as 2128ppm (7660 mg/m³) based on increased resorptions and NOAEL = 597ppm (2150mg/m³) (Dalbey *et al.*, 1996a,b).

8 HUMAN EXPOSURE SUMMARY

There are no studies available that monitor the exposure of workers or the public to the members of the LOF category because these materials are primarily site-limited to refinery pipelines and are blended directly into gasoline.

9 TEST PLAN SUMMARY

The data presented in this test plan are adequate to characterize selected HPV Program endpoints for the LOF Category. Since the LOF Category substances are composed of branched paraffins and olefins, the available toxicity data for two similar streams, Mixed LOF, and Light Catalytically Cracked Naphtha (LCCN), are ideal for evaluating the toxicity of the LOF Category. Due to the robustness of the LCCN dataset, no additional testing for the Light Oxo Fraction Category is proposed.

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APPENDIX A – LOF REACH REGISTRATION

**APPENDIX B – GASOLINE BELNDING STREAMS CATEGORY ASSESSMENT
DOCUMENT**

201-16863B

Description: Description: C:\Users\malampi\Desktop\iuclid5.jpg

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2011 SEP -6 PM 1:01

Printing Date 2011-08-31 10:02:11 CEST

Restriction of specific regulatory purposes

EU: BPD, EU: PPP, EU: REACH, CA: CEPA, CA: PCPA, JP: CSCL, OECD: HPVC, US: EPA HPVC, US: FIFRA, US: TSCA, other:

Confidentiality

Name Mixed LOF

Substance: Mixed LOF

UUID IUC5-78a1730d-e4de-4804-a4fa-61ee8ae909dc
Dossier 0
UUID

Date 2010-09-21 09:54:13 CEST

Remarks

1 General Information

1.1 Identification

Substance identification

Chemical name Mixed LOF

EU: REACH

Legal entity [ExxonMobil Chemical Holland B.V. / Botlek / Netherlands](#)

EU: REACH

Role in the supply chain

EU: REACH

Role: Manufacturer

Reference substance

[Alkenes, C6-10, hydroformylation products, low-boiling / None available - not a single isomer - see remarks](#)

EC number **EC name**

CAS number **CAS name**

IUPAC name

None available - not a single isomer - see remarks

Type of substance

Composition UVCB

Origin organic

Trade names

EU: REACH

Name Mixed LOF

Name Alkenes, C6-10, hydroformylation products, low-boiling

4 Physical and chemical properties

4.1 Appearance/physical state/colour

Endpoint study record: Appearance/physical state/colour.001

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Dossier UUID 0
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Date 2010-07-28 13:49:25 CEST
Remarks Successfully migrated to IUCLID 5.2 format.

Administrative Data

EU: REACH

Purpose flag	key study; robust study summary
Study result type	experimental result Study period 2010
Reliability	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies	Standard test method followed, no GLP laboratory.

Data source

Reference

Reference type	Author	Year	Title	Bibliographic source	Testing laboratory	Report no.	Owner company	Company study no.	Report date
study report	ExxonMobil Chemical	2010	Colour measurement on LOF		ExxonMobil Chemical, MCTC laboratory, Machelen, Belgium	MAC 201004.0197	ExxonMobil Chemical	MAC 201004.0197	

Data access

data submitter is data owner

Data protection claimed

yes, but willing to share

Materials and methods

Test guideline

Qualifier	Guideline	Deviations
according to	other guideline: ASTM D 1209	no

GLP compliance

no (none GLP lab)

Test materials

Identity of test material same as for substance defined in section 1 (if not read-across)

yes

Test material identity

Identifier	Identity
Common name	Alkenes, C6-10, hydroformylation products, low-boiling

Details on test material

Commercial grade

Results and discussion

Physical state at 20°C and 1013 hPa

liquid

Form

other: moderate viscosity

Colour

5 on PtCo scale (yellow)

Odour

other: Petroleum odour

Substance type

organic

Applicant's summary and conclusion

Conclusions

Mixed LOF is a colourless to yellow liquid with a petroleum odour at 20°C.

Executive summary

Mixed LOF is a colourless to yellow liquid with a petroleum odour at 20°C.

4.3 Boiling point

Endpoint study record: Boiling point.001

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Dossier 0
UUID
Author XML Transformation V1.0 Plug-In
Date 2010-07-28 13:54:14 CEST
Remarks Successfully migrated to IUCLID 5.2 format.

Administrative Data

EU: REACH

Purpose flag	key study; robust study summary
Study result type	experimental result Study period 2010
Reliability	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies	According standard test method no GLP lab

Data source

Reference

Reference type	Author	Year	Title	Bibliographic source	Testing laboratory	Report no.	Owner company	Company study no.	Report date
study report	ExxonMobil Chemical	2010	GCD analysis on Mixed LOF.		ExxonMobil Chemical, MCTC laboratory, Machelen, Belgium	MAC 201004.0197	ExxonMobil Chemical	MAC 201004.0197	

Data access

data submitter is data owner

Data protection claimed

yes

Materials and methods

Test guideline

Qualifier	Guideline	Deviations
according to	other guideline: ASTM D 2887	no

Type of method

other: GCD

GLP compliance

no (None GLP lab)

Test materials

Identity of test material same as for substance defined in section 1 (if not read-across)

yes

Test material identity

Identifier	Identity
Common name	Alkenes, C6-10, hydroformylation products, low-boiling

Details on test material

Commercial grade

Results and discussions

Boiling point

Boiling pt.	Atm. pressure	Decomposition	Decomp. temp.	Remarks
102 — 182 °C	1 atm	no		

Applicant's summary and conclusion

Conclusions

Measured boiling range for Mixed LOF with GCD is 102 to 182°C with ASTM D 2887.

Executive summary

Measured boiling range for Mixed LOF with GCD is 102 to 182°C with ASTM D 2887.

4.6 Vapour pressure

Endpoint study record: Vapour pressure.001

UUID IUC5-13696e44-780d-4276-a33b-
f3a1dcb959a1

**Dossier
UUID** 0

Date 2010-09-17 15:41:34 CEST

Remarks

Administrative Data

EU: REACH

Purpose flag	weight of evidence
Study result type	estimated by calculation Study period 2010
Reliability	2 (reliable with restrictions)
Rationale for reliability incl. deficiencies	Calculated values

Data source

Reference

Reference type	Author	Year	Title	Bibliographic source	Testing laboratory	Report no.	Owner company	Company study no.	Report date
other company data	ExxonMobil Chemical	2010	vapour pressure	Brandes-Möller, 2008, Verlag für neue Wissenschaft GmbH, Bremerhaven			ExxonMobil Chemical		2010-02-02

Data access

data submitter is data owner

Data protection claimed

yes, but willing to share

Materials and methods

Test guideline

Qualifier	Guideline	Deviations
no guideline followed	other guideline: extrapolated from published data	

Type of method

other: extrapolated from published data

Principles of method if other than guideline

Read-across from typical alkane isomers - e.g. 2,3 dimethylhexane .

(Safety Characteristic Data, Brandes-Möller, 2008, Verlag für neue Wissenschaft GmbH, Bremerhaven).

GLP compliance

no (extrapolated data)

Test materials

Identity of test material same as for substance defined in section 1 (if not read-across)

yes

Test material identity

Identifier	Identity
IUPAC name	None available - not a single isomer - see remarks

Results and discussions

Vapour pressure

< 20 kPa

50 °C

Transition / decomposition

**Transition / no
decomposition**

Applicant's summary and conclusion

Conclusions

The extrapolated vapour pressure is below 20 kPa at 50°C.

Executive summary

The extrapolated vapour pressure is below 20 kPa at 50°C.

5 Environmental fate and pathways

5.2 Biodegradation

5.2.1 Biodegradation in water: screening tests

***Endpoint study record: Biodegradation in water: screening tests/EM
(1996)/Mixed LOF/k***

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UUID

Date 2010-09-21 21:49:27 CEST

Remarks

Administrative Data

EU: REACH

Purpose flag key study

Study result type experimental result

Reliability 1 (reliable without restriction)

Data source

Reference

Reference type	Author	Year	Title	Bibliographic source	Testing laboratory	Report no.	Owner company	Company study no.	Report date
study report	ExxonMobil Biomedical Sciences, Inc.	1997	Ready Biodegradability: OECD 301F Manometric Respirometry Test		ExxonMobil Biomedical Sciences, Inc	146194A	ExxonMobil Chemical Company		

Data access

data submitter is data owner

Data protection claimed

yes, but willing to share

Materials and methods

Test type

ready biodegradability

Test guideline

Qualifier	Guideline	Deviations
according to	OECD Guideline 301 F (Ready Biodegradability: Manometric Respirometry Test)	no

GLP compliance

yes

Test materials

Identity of test material same as for substance defined in section 1 (if not read-across)

yes

Test material identity

Identifier	Identity
Common name	Mixed LOF

Study design

Oxygen conditions

aerobic

Inoculum or test system

activated sludge, non-adapted

Details on inoculum

Activated sludge was obtained from the Somerset-Raritan Valley Sewage Authority in Bridgewater, NJ, USA.

Duration of test (contact time)

28 d

Initial test substance concentration

Initial conc.	Based on
ca. 41 mg/L	test mat.

Parameter followed for biodegradation estimation

CO2 evolution

Reference substance

benzoic acid, sodium salt

Results and discussions

% Degradation of test substance

%Degr.	St. dev.	Parameter	Sampling time	Remarks
52		CO2 evolution	28 d	

BOD5 / COD results

Results with reference substance

Sodium benzoate degraded >60% by day 14, and fulfilled guideline requirement.

Overall remarks, attachments

Overall remarks

52% biodegradation of mixed LOF was observed after 28 d in an OECD 301F ready biodegradability test, indicating the substance is inherently biodegradable.

Applicant's summary and conclusion

Validity criteria fulfilled

yes

Interpretation of results

inherently biodegradable

Conclusions

52% biodegradation of mixed LOF was observed after 28 d in an OECD 301F ready biodegradability test, indicating the substance is inherently biodegradable.

Executive summary

52% biodegradation of mixed LOF was observed after 28 d in an OECD 301F ready biodegradability test, indicating the substance is inherently biodegradable.

6 Ecotoxicological Information

6.1 Aquatic toxicity

6.1.1 Short-term toxicity to fish

Endpoint study record: Short-term toxicity to fish/Mixed LOF/EM1996/k

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UUID** 0

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Remarks

Administrative Data

EU: REACH

Purpose flag key study

Study result type experimental result

Reliability 1 (reliable without restriction)

Data source

Reference

Reference type	Author	Year	Title	Bibliographic source	Testing laboratory	Report no.	Owner company	Company study no.	Report date
study report	ExxonMobil	1996	Fish, Acute Toxicity Test, Rainbow Trout-Renewal		ExxonMobil Biomedical Sciences, Inc	146158	ExxonMobil Chemical Company		

Data access

data submitter is data owner

Data protection claimed

yes, but willing to share

Materials and methods

Test guideline

Qualifier	Guideline	Deviations
according to	OECD Guideline 203 (Fish, Acute Toxicity Test)	no

GLP compliance

yes

Test materials

Identity of test material same as for substance defined in section 1 (if not read-across)

yes

Test material identity

Identifier	Identity
Common name	Mixed LOF

Analytical monitoring

yes

Details on sampling

Samples were taken on Day 0, 1, 2, and 3 from the stirring vessels used to prepare the WAFs and from the 'old' WAFs of each treatment on Day 1 and at termination for analysis.

Vehicle

no

Details on test solutions

Test solution was renewed daily.

Test organisms

Test organisms (species)

Oncorhynchus mykiss

Details on test organisms

Fish were approximately 4 weeks old at initiation of exposure, and were quarantined and observed for parasites and disease for at least 12 days before the test.

Study design

Test type

semi-static

Water media type

freshwater

Limit test

no

Total exposure duration

96 h

Test conditions

Test temperature

15 C

Results and discussions

Effect concentrations

Duration	Endpoint	Effect conc.	Nominal/Measured	Conc. based on	Basis for effect	Remarks (e.g. 95% CL)
96 h	LL50	21 mg/L	meas. (arithm. mean)	test mat.	mortality	

Overall remarks, attachments

Overall remarks

In an exposure to WAFs of Mixed LOF to rainbow trout, the 96-hour LL50 was calculated to be 21 mg/L.

Applicant's summary and conclusion

Conclusions

In an exposure to WAFs of Mixed LOF to rainbow trout, the 96-hour LL50 was calculated to be 21 mg/L.

Executive summary

In an exposure to WAFs of Mixed LOF to rainbow trout, the 96-hour LL50 was calculated to be 21 mg/L.

