March 27, 2003

Steven A. Signs, Ph.D., D.A.B.T.
Technical Contact
The Lubrizol Corporation
29400 Lakeland Boulevard
Wickliffe, OH 44092

Dear Dr. Signs:

The Office of Pollution Prevention and Toxics is transmitting EPA's comments on the robust summaries and test plan for Petroleum Oxidates and Derivatives Thereof Category posted on the ChemRTK HPV Challenge Program Web site on November 27, 2002. I commend The Lubrizol Corporation for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that The Lubrizol Corporation advise the Agency, within 90 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the "Contact Us" link on the HPV Challenge Program Web site pages or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

-S-

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: C. Auer
A. Abramson
W. Penberthy
M. E. Weber

EPA Comments on Chemical RTK HPV Challenge Submission:
Petroleum Oxidates and Derivatives Thereof Category

SUMMARY OF EPA COMMENTS

The sponsor, The Lubrizol Corporation, submitted a test plan and robust summaries to EPA for the Petroleum Oxidates and Derivatives Thereof Category dated November 11, 2002. EPA posted the submission on the ChemRTK HPV Challenge Web site on November 27, 2002.

EPA has reviewed this submission and has reached the following conclusions:

1. Category Justification. While the justification provided for grouping the seven members of the proposed second subcategory is reasonable, the submitter's plan to apply "read across" extrapolation between the subcategories for the repeated-dose, reproductive and developmental toxicity endpoints is not justified because the two subcategories differ significantly in molecular weight range, carbon chain length, and physicochemical properties.

2. Physicochemical Properties. The data provided by the submitter for melting point, boiling point, vapor pressure, partition coefficient, and water solubility are adequate for the purposes of the HPV Challenge Program. The test plan needs to specify read-across extrapolation as the intended route to physicochemical data for CAS No. 68603-12-3.

3. Environmental Fate. The submitter's plan to provide data for photodegradation and fugacity is adequate for the purposes of the HPV Challenge Program. Although the test plan states that these substances do not undergo hydrolysis, robust summaries stating the rationale are needed. The submitter also needs to provide biodegradation data for at least three substances in subcategory 2.

4. Health Effects. The submitted gene mutation data are inadequate for the purposes of the HPV Challenge Program. The submitter therefore needs to provide additional data for this endpoint. EPA agrees with the submitter's plan to test CAS No. 64742-98-9 for repeated-dose, genetic (chromosomal aberrations), and reproductive/developmental toxicity for subcategory 1, but disagrees with the proposed acute toxicity testing protocol. In addition to the proposed chromosomal aberrations test for subcategory 2, EPA recommends testing CAS No. 64743-00-6 for repeated-dose, reproductive and developmental toxicity.

5. Ecological Effects. EPA agrees with the submitter's proposal to conduct acute tests of oxidized light distillate (petroleum) [CAS No. 64742-98-9] in fish, aquatic invertebrates and aquatic plants. EPA also recommends a daphnia chronic study because of the high carbon chain component in this substance. The data submitted for the substances in subcategory 2 are adequate for the purposes of the HPV Challenge Program.

EPA requests that the submitter advise the Agency within 90 days of any modifications to its submission.

EPA COMMENTS ON THE PETROLEUM OXIDATES AND DERIVATIVES THEREOF CATEGORY CHALLENGE SUBMISSION

Category Definition

The submitter proposes a category covering eight substances produced from the oxidation of petroleum distillates, slack wax, and petrolatum. Category members are divided into two subcategories based on the molecular weight range of the starting materials.

Subcategory 1 consists of one substance, oxidized light distillates (petroleum) [CAS No. 64742-98-9]. This substance is derived from aliphatic hydrocarbons with carbon numbers ranging from C9-C16. The oxidized product is composed of 50% unreacted hydrocarbons, 25% ketones, 10% mono- and dicarboxylic acids, and the remaining 15% of the substance consisting of oxyacids, aldehydes and methyl esters.

Subcategory 2 contains seven members that are derived from the oxidation of slack wax or petrolatum streams and contains aliphatic hydrocarbons ranging in carbon number from C33-C43. The submitter reports that the substances, oxidized hydrocarbon waxes (petroleum) [CAS No. 64743-00-6] and oxidized petrolatum (petroleum) [CAS No. 64743-01-7], contain 40-50% unreacted hydrocarbons from the starting material and 30-35% monocarboxylic acids, with the remaining 15-30% of these substances containing dicarboxylic acids, oxyacids, aldehydes and ketones. The other substances in subcategory 2 are derivatives of the oxidized hydrocarbon wax and petrolatum substances. In these substances, a fraction of the carboxylic acids are either converted to a salt [oxidized petrolatum (petroleum), calcium salt] [CAS No. 69425-34-3], derivatized to the methyl ester [oxidized hydrocarbon waxes (petroleum), methyl ester] [CAS No. 68602-85-7], or transformed to the methyl ester salt through the reaction of the unesterified carboxylic acids with barium [oxidized hydrocarbon waxes (petroleum), methyl ester, barium salts] [CAS No. 68603-10-1], calcium [oxidized hydrocarbon waxes (petroleum), methyl ester, calcium salts] [CAS No. 68603-11-2], or sodium ions [oxidized hydrocarbon waxes (petroleum), methyl ester, sodium salts] [CAS No. 68603-12-3].

Category Justification

The submitter states that category members are divided into two subcategories due to apparent differences in physicochemical properties between the oxidates derived from petroleum distillates and those derived from slack wax or petrolatum. EPA disagrees with grouping these two subcategories into one category because the differences in molecular weight range, carbon chain length, and physicochemical properties are substantial. However, grouping the seven members of subcategory 2 is supported by physicochemical data and chemical composition. The submitter proposes testing members of both subcategories for environmental fate, ecotoxicity and genotoxicity, but to apply “read across” extrapolation from subcategory 1 to 2 for the repeated-dose, reproductive and developmental toxicity endpoints. This extrapolation is based on the submitter’s assumption that subcategory 1 represents the upper bound of toxicity for the overall category because it has lower molecular weight members and is therefore more bioavailable. EPA believes that the structure and property differences cited above are too great to justify this approach.

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient and water solubility). The data provided by the submitter for melting point, boiling point, vapor pressure, partition coefficient, and water solubility are adequate for the purposes of the HPV Challenge Program. The submitter needs to state in the test plan that “read across” extrapolation from other subcategory members will be used to estimate physicochemical values for CAS No. 68603-12-3

Water solubility. On page 5 of the test plan, the submitter indicates that the petroleum oxidates in category 2 have a water solubility range of 0.35 to 1.29 ***ppb***. However, in Table 1 (page 6), the values range from 0.35 to 1.29 ***ppm***. The units used in the robust summary for water solubility are in ***ppb***. The submitter needs to correct these discrepancies. Using the same units in the robust summary as in the test plan would avoid confusion.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity).

Stability in water. To justify no additional testing, the submitter states that these substances will not undergo significant hydrolysis. EPA agrees with the submitter's reasoning. However, the submitter needs to include this reasoning in robust summaries for this endpoint.

Biodegradation. The submitter indicates that biodegradation data will be provided for CAS No. 64742-98-9 (in subcategory 1) and 64743-00-6 (in subcategory 2). Testing only one member of subcategory 2 is not sufficient to characterize biodegradation for all chemicals in this subcategory. It is not the objective of the HPV Challenge Program to obtain data on the "most biodegradable" substance in the category, but on as many substances as needed to adequately represent the category. Therefore, the submitter needs to provide biodegradation data on at least the following three substances: CAS No. 64742-98-9; 64743-00-6; and 68603-11-2. Although pure compounds are preferred for biodegradation tests, when a mixture is tested the submitter needs to provide biodegradation rate information on the components of the mixture that have biodegraded over the study period because some components may be more biodegradable than others.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive/developmental toxicity).

EPA agrees with the submitter's plan to test light oxidized petroleum distillates (CAS No. 64742-98-9), the sole member of subcategory 1, for repeated-dose, genetic (chromosomal aberrations), and reproductive/ developmental toxicity, but disagrees with the proposed acute toxicity test protocol. EPA recommends testing the acute oral toxicity endpoint by following OECD TG 425, the up-and-down procedure, unless the submitter can provide a rationale for using a different OECD protocol, such as OECD TG 423. In addition to the proposed chromosomal aberrations test for subcategory 2, testing is needed on a member of subcategory 2, such as oxidized petroleum hydrocarbon waxes (CAS No. 64743-00-6), for repeated-dose, reproductive and developmental toxicity, following OECD TG 422. Testing a member of subcategory 2 for these endpoints is needed because of the differences in molecular weight range and carbon chain length, as well as physicochemical properties, between the members of subcategory 1 and subcategory 2.

Acute Toxicity. In Table 5 of the test plan, "read across" extrapolation is proposed for the acute mammalian toxicity of CAS No. 68603-10-1. However, acute toxicity data are available for this petroleum oxidate according to Table 4 of the test plan. The submitter needs to correct this error.

Genetic Toxicity. The submitted mutagenicity data are not adequate for the purposes of the HPV Challenge Program because only one bacterial strain was tested. The submitter needs to provide additional bacterial mutation data.

Ecological Effects (fish, invertebrates, and algae).

EPA recommends a chronic toxicity study in daphnia for oxidized light distillate (petroleum) [CAS No. 64742-98-9] because of the high carbon chain length component in this substance. Also, the submitter indicated that the calculated octanol water partition coefficient (log Kow) of CAS No. 64742-98-9 is between 3.3 and 7.06. EPA believes that components in chemical mixtures having a log Kow of $\geq$4.2 -7.0 are likely to exhibit chronic toxicity. Chronic toxicity testing should be conducted using a flow-through method with measured concentrations at or below the water solubility limit. Because the substance has a low water solubility, the Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures should be followed (http://www.oecd.org./ehs/test/monos.htm).

Although acute tests were conducted with subcategory 2 substances above water solubility limits, the data are adequate for the purposes of the HPV Challenge Program. In general, chemicals with a high log Kow (>7.0) and low water solubility do not exhibit acute or chronic toxicity to aquatic organisms.

Specific Comments on the Robust Summaries

Health Effects

Acute Toxicity. The robust summaries for CAS Nos. 64743-00-6 and CAS No. 68603-10-1 do not include mortality data.

Followup Activity

EPA requests that the submitter advise the Agency within 90 days of any modifications to its submission.