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11/18/2009 02:09 PM

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Subject HPV submission for Stepan: CAS 3088-31-1

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11/17/2009 01:17 PM

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Subject HPV submission for Stepan: CAS 3088-31-1

Attached please find the revised Chemical RTK HPV Challenge Submission for Sodium 2-(2-Dodecyloxyethoxy)ethyl Sulfate, CAS No 3088-31-1. These documents have been revised in response to EPA comments received on the original test plan submission. The submitted documents include a revised Test Plan, dossier and responses to EPA comments.

If you have any questions please contact me or the sponsor representative:

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Thank you.

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3088-31-1 Nov 5 2009.rtf SN403 SLS EPA Comments 110509.doc TestPlanCAS3088311_November_05_2009.doc

EPA Comments on Chemical RTK HPV Challenge Submission
Sodium 2-(2-Dodecyloxyethoxy)ethyl Sulfate

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SUMMARY OF EPA COMMENTS

The sponsor, Stepan Company, submitted a test plan and robust summaries to EPA for Sodium 2-(2-dodecyloxyethoxy)ethyl sulfate dated July 12, 2006 and revised summaries on September 18, 2006. EPA posted the submission on the Chem RTK HPV Challenge Web site on October 20, 2006 and posted the revised summaries on March 8, 2007. Data on the analog substances sodium lauryl ether sulfate (SLES; CAS No. 9004-82-4) and the alcohol ethoxysulfates (AES) category were also submitted.

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

1. Analog Justification. For human health and ecological endpoints, the analog justification appears adequate. For the human health endpoints, EPA did not consider data on mixtures comprised of more than one CAS-numbered substance or on substances with counter-ions other than sodium to be appropriate to characterize the sponsored substance. Noted.
2. Physical Chemical Properties. There are adequate data for boiling point, vapor pressure, water solubility, and log K_{ow} for the purposes of the HPV Challenge Program. The melting point data are inadequate. A measured melting point for the sponsored substance has been provided.
3. Environmental Fate. There are adequate data for these endpoints for the purposes of the HPV Challenge Program. Noted.
4. Health Effects. Adequate data were submitted on either the sponsored substance or the analog substances to address all SIDS endpoints for the purposes of the HPV Challenge Program. The submitter needs to address deficiencies in the robust summaries. Agree.
5. Ecological Effects. EPA reserves judgment on the adequacy of the data submitted for acute fish and invertebrates pending submission of critical data elements missing from the robust summaries. Algal data submitted were not adequate for the purposes of the HPV Challenge Program and data need to be provided to satisfy this endpoint. Chronic daphnia data summaries need more details. See detailed response below.

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

**EPA COMMENTS ON THE SODIUM 2-(2-DODECYLOXYETHOXY)ETHYL SULFATE
CHALLENGE SUBMISSION**

Analog Justification

The submitter proposes using data for sodium lauryl ether sulfate (SLES; CAS No. 9004-82-4) and other members of an alcohol ethoxysulfates (AES) category to read across to the sponsored substance primarily on the basis of similarities in structure. The AES category comprises commercial grades of linear-type primary alcohol ethoxysulfates containing AES components of basic structure $C_nH_{2n+1}O(C_2H_4O)_mSO_3X$ where $n=10-18$ and $m=0-8$ and X =sodium, ammonium or triethanolammonium ion. The submitter states that sodium laureth sulfate is within this definition. In addition to SLES, the following substances (all mixtures of related substances) are members of the analogous category:

<u>CAS Number</u>	<u>CAS Description</u>
27028-82-6	Ethanol, 2,2',2''-nitrilotris-, compd. with α -sulfo- ω -(dodecyloxy)poly(oxy-1,2-ethanediyl) (1:1)
54116-08-4	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -tridecyloxy-, sodium salt
67762-19-0	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C10-16-alkyl ethers, ammonium salts
68037-05-8	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C6-10-alkyl ethers, ammonium salts
68037-06-9	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C6-10-alkyl ethers
68540-47-6	Ethanol, 2,2',2''-nitrilotris-, compd. with α -sulfo- ω -(tetradecyloxy)poly(oxy-1,2-ethanediyl) (1:1)
68585-34-2	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C10-16-alkyl ethers, sodium salts
68585-40-0	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C16-18-alkyl ethers, sodium salts
68891-38-3	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C12-14-alkyl ethers, sodium salts
96130-61-9	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C9-11-alkyl ethers, sodium salts
105859-96-9	Ethanol, 2,2',2''-nitrilotris-, compds. with polyethylene glycol hydrogen sulfate C11-15-sec-alkyl ether ammonium salts
125301-92-0	Poly(oxy-1,2-ethanediyl), α -sulfo- ω -hydroxy-, C12-15-alkyl ethers, sodium salts
125304-06-5	Ethanol, 2,2',2''-nitrilotris-, compds. with polyethylene glycol hydrogen sulfate C16-18-alkyl ether
129783-23-9	Ethanol, 2,2'-iminobis-, compds. with polyethylene glycol hydrogen sulfate C12-15-alkyl ethers
157627-92-4	Alcohols, C10-16, ethoxylated, sulfates, mono(hydroxyethyl)ammonium salts (>1 <2.5 mol EO)
157707-82-9	Alcohols, C14-16, ethoxylated, sulfates, sodium salts (>1 <2.5 mol EO)
162201-45-8	Ethanol, 2-amino-, compds. with polyethylene glycol hydrogen sulfate C12-15-alkyl ethers

In the data summaries, a structure code rather than a CAS number is used to describe the test substances.

For the human health endpoints, EPA did not consider data on complex mixtures (those comprised of more than one CAS-numbered substance) or substances with counter-ions other than sodium to be appropriate to characterize the sponsored substance. The ammonium and triethanolammonium counter-ions have intrinsic chemical properties that add a level of complexity not representative of the sponsored substance. The limited data submitted for the sponsored substance suggest that it is less toxic than the analog substances. From structural similarities and the limited data for the sponsored substance, the use of selected analog data appears adequate for the purposes of the HPV Challenge Program.

Test Plan

Physicochemical Properties (melting point, boiling point, vapor pressure, partition coefficient, water solubility)

There are adequate data for boiling point, vapor pressure, water solubility, and log K_{ow} for the purposes of the HPV Challenge Program. The melting point data are inadequate. **A measured melting point for the sponsored substance has been provided.**

Melting point. The submitter provided an estimated (MPBPWIN v 1.41) for the sponsored substance. Estimated melting points are not adequate for the HPV Program. According to HPV Guidelines, the melting or decomposition point for a chemical substance should be determined experimentally unless the melting point is less than 0 EC. The submitted data for this endpoint are inadequate. **A measured melting point value for the sponsored substance has been provided.**

Water solubility. The test compound is a strong surfactant and measurement of its water solubility would be both difficult and unlikely to provide further useful information. The submitted data are adequate. **Noted.**

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

There are adequate data for these endpoints for the purposes of the HPV Challenge Program. **Noted**

Biodegradation. The submitter provided data from OECD TG 306 for the sponsored substance. While this is not strictly an aerobic ready biodegradation test, a positive result from this test is generally considered to indicate ready biodegradability, as biodegradation in seawater is considered to be slower than in an environment containing activated sludge or sewage. Analog data are in good agreement with the results obtained for the sponsored substance and the data are adequate for this endpoint **Noted.**

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

Adequate data were submitted on either the sponsored substance or the analog substances to characterize all SIDS endpoints for the purposes of the HPV Challenge Program. The submitter needs to address deficiencies in the robust summaries. **Agree to provide additional, available data as requested.**

The summaries for analog substances will be provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance once they become available.

General. The data for the repeated-dose, genetic and reproductive/developmental toxicity endpoints were submitted as a summary document. Even after EPA referred the submitter to the guidance document on preparing robust summaries (<http://www.epa.gov/chemrtk/pubs/general/robsumgd.htm>), the revised summaries had limited study details, which hindered the independent evaluation of the relevant data. The purity and identity of the analog substance is not always clear and should be clarified in the revised summaries, which should preferably be in IUCLID format. **Agree to provide additional, available details as requested. The summaries for analog substances will be provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance(s) once they become available.**

Genetic Toxicity (Chromosomal Aberrations). Data submitted for AES substances NaC12-15AES, NaC12-15E3S and C12-13E2.5S appear adequate to address this endpoint, using a weight-of-evidence approach because the methodology was not described in much detail. **Noted.**

Ecological Effects (fish, invertebrates, and algae)

EPA reserves judgment on the adequacy of the data submitted for acute fish and invertebrate tests for key analogs pending submission of missing critical data elements (see Specific Comments below). Algal data submitted were not adequate and data need to be provided to satisfy this endpoint. Chronic daphnia data submitted need to be enhanced with robust summary details to help interpret test results.

Algae. Tests were not conducted within the required 96/72-h duration. The submitter needs to provide adequate measured data, or estimated data plus measured data on an appropriate analog for this endpoint. Agree to provide additional, available details as requested. The summaries for analog substances will be provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance(s) once they become available.

Invertebrates (Chronic). The 21-d *D. magna* reproduction and NOEC study results (Scholz, 1997, BKH 1994, and BUA 1997) in Table 11 of the HERA AES Environmental Risk Assessment document need to be submitted in robust summary format to be useful for the purposes of the HPV Challenge program. Agree to add details from Table 11 of the HERA AES Environmental Risk Assessment document to the dossier. However, details for reliable robust summaries will not be available until the summaries for analog substances are provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance(s) once they become available.

Specific Comments on the Robust Summaries

General

The robust summaries for health and ecological effects lack sufficient detail for the purposes of the HPV Challenge program. The submitter needs to review the EPA guidance for developing robust summaries (<http://www.epa.gov/chemrtk/pubs/general/robsumgd.htm>) and enhance the summaries accordingly. The reliability needs to be given a value to complement the written evaluation according to Klimisch et al. (1997). It would be helpful if the analog data were submitted in IUCLID format to address the information commonly provided (e.g. purity of the test substance, description of methodology and results) in robust summaries to allow an independent evaluation of the submitted data.

Ecological Effects

Fish. The fish 96-h study summary (*Pimephales promelas*, LC₅₀ value of 13 mg/L) needs to be enhanced to include CAS No. of test substance, number of ethoxy groups present, whether test used nominal or measured concentrations, test method, number of organisms per test, number of replicates, and dissolved oxygen content. Agree to provide additional, available details as requested. The summaries for analog substances will be provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance(s) once they become available.

Invertebrates. The *Ceriodaphnia dubia* 48-h study summary (EC₅₀ value of 3.12 mg/L) needs to be enhanced to include pH, water hardness, dissolved oxygen content, number of replicates, number of organisms per replicate, measured or nominal concentrations, and test method. Agree to provide additional, available details as requested. The summaries for analog substances will be provided by the REACH Consortium Linear and Branched AES (C₁₀ – C₁₆) and will be added to the IUCLID dossier for the sponsored substance(s) once they become available.

Followup Activity

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

References

Klimisch, H-J, Andreae, M and Tillmann, U. (1997) A systematic approach for evaluation the quality of experimental toxicological and ecotoxicological data. *Regul. Toxicol. Pharmacol.* 25:1-5.