SCREENING-LEVEL HAZARD CHARACTERIZATION

Aldehydes, C4, Self-Condensation Products, High-Boiling Fraction (CASRN 68990-21-6)

The High Production Volume (HPV) Challenge Program[1] was conceived as a voluntary initiative aimed at developing and making publicly available screening-level health and environmental effects information on chemicals manufactured in or imported into the United States in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsored chemicals; sponsorship entailed the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data did not exist, and making both new and existing data and information available to the public. Each complete data submission contains data on 18 internationally agreed to "SIDS" (Screening Information Data Set[1,2]) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1400 sponsored chemicals by developing hazard characterizations (HCs). These HCs consist of an evaluation of the quality and completeness of the data set provided in the Challenge Program submissions. They are not intended to be definitive statements regarding the possibility of unreasonable risk of injury to health or the environment.

The evaluation is performed according to established EPA guidance[2,3] and is based primarily on hazard data provided by sponsors; however, in preparing the hazard characterization, EPA considered its own comments and public comments on the original submission as well as the sponsor's responses to comments and revisions made to the submission. In order to determine whether any new hazard information was developed since the time of the HPV submission, a search of the following databases was made from one year prior to the date of the HPV Challenge submission to the present: (ChemID to locate available data sources including Medline/PubMed, Toxline, HSDB, IRIS, NTP, ATSDR, IARC, EXTOXNET, EPA SRS, etc.), STN/CAS online databases (Registry file for locators, ChemAbs for toxicology data, RTECS, Merck, etc.) and Science Direct. OPPT's focus on these specific sources is based on their being of high quality, highly relevant to hazard characterization, and publicly available.

OPPT does not develop HCs for those HPV chemicals which have already been assessed internationally through the HPV program of the Organization for Economic Cooperation and Development (OECD) and for which Screening Initial Data Set (SIDS) Initial Assessment Reports (SIAR) and SIDS Initial Assessment Profiles (SIAP) are available. These documents are presented in an international forum that involves review and endorsement by governmental authorities around the world. OPPT is an active participant in these meetings and accepts these documents as reliable screening-level hazard assessments.

[1] U.S. EPA. High Production Volume (HPV) Challenge Program; http://www.epa.gov/chemrtk/index.htm.
[2] U.S. EPA. HPV Challenge Program – Information Sources; http://www.epa.gov/chemrtk/pubs/general/guidocs.htm.
[3] U.S. EPA. Risk Assessment Guidelines; http://cfpub.epa.gov/ncea/raf/rafguid.cfm.

These hazard characterizations are technical documents intended to inform subsequent decisions and actions by OPPT. Accordingly, the documents are not written with the goal of informing the general public. However, they do provide a vehicle for public access to a concise assessment of the raw technical data on HPV chemicals and provide information previously not readily available to the public.

Chemical Abstract Service Registry Number (CASRN)	**68990-21-6**
Chemical Abstract Index Name	Aldehydes, C4, self-condensation products, high-boiling fraction
Structural Formula	**Mixture**

Summary

EPA reviewed the submission for CASRN 68990-21-6 and determined that the chemical composition proposed by the sponsor requires analytical verification. In the absence of this information, only submitted information on CASRN 68990-21-6 was considered in this hazard characterization.

The physical-chemical properties and environmental exposure and fate for CASRN 68990-21-6 could not be determined because no data are available.

The potential health hazard of CASRN 68990-21-6 cannot be evaluated because no data are available.

The potential hazard to the environment of CASRN 68990-21-6 cannot be evaluated because no data are available.

All SIDS endpoints are identified as data gaps under the HPV Challenge Program.

The sponsor, Eastman Chemical Company, submitted a Test Plan and a table to EPA for aldehydes, C4, self-condensation products, high-boiling fraction (Solvent C; CASRN 68990-21-6; CA Index name: aldehydes, C4, self-condensation products, high-boiling fraction) on August 26, 2002. EPA posted the submission on the ChemRTK HPV Challenge website on September 23, 2002 (http://www.epa.gov/HPV/pubs/summaries/c4aldehy/c13949tc.htm). EPA comments on the original submission were posted to the website on January 21, 2003. Public comments were also received and posted to the website. The sponsor submitted updated/revised documents on February 5, 2003, which were posted to the ChemRTK website on February 12, 2003.

Justification for Supporting Chemicals

The sponsored substance (aldehydes, C4 self-condensation products, high boiling fraction, CASRN 68990-21-6, also called Solvent C) is a Class 2[4] substance which is formed by combining the waste streams from four different manufacturing processes. These processes were not identified by the sponsor. The sponsor proposed that the following chemical components of Solvent C were appropriate supporting chemicals: di-2-ethylhexyl ether, CASRN 10143-60-9; butyl butyrate, CASRN 109-21-7; neopentyl glycol, CASRN 126-30-7; 2,2,4-trimethyl-1,3-pentanediol, CASRN 144-19-4; n-butyl alcohol, CASRN 71-36-3; 2-ethyl-1,3-hexanediol, CASRN 94-96-2; 2-ethylhexanol, CASRN 104-76-7; isobutyl alcohol, CASRN 78-83-1; isobutyl isobutyrate, CASRN 97-85-8; and butyric acid, CASRN 107-92-6). The sponsor also indicated that Solvent C contains 2 – 10% alkyl acetals (No CASRN), formed by a reaction between alcohols and aldehydes. In both the initial test plan and the revised test plan, the sponsor indicated that existing data on these chemicals should be used to satisfy the SIDS endpoints; however, the sponsor did not submit robust summaries for these data.

EPA comments posted January 21, 2003 provided the following major reasons as to why EPA was unable to continue its evaluation of the initial test plan submission: (1) The sponsor did not provide an analytical description of the components of a representative sample of Solvent C; (2) The test plan stated "Since Solvent C consists of many chemicals present in varying amounts it is not known how the various SIDS endpoints will be affected by their presence as a mixture." EPA noted in their comments that this suggests that testing the mixture may be the preferred option, but no further characterization of the mixture and no Robust Summaries were provided in the revised submission; and (3) The test plan did not summarize hazard information for the components of Solvent C.

EPA has determined that the information provided by the sponsor for Solvent C is inadequate for human health hazard and aquatic toxicity assessment for the following reasons: (1) The sponsor did not provide an analytical description of the components of a representative sample of Solvent C; (2) The data which the sponsor wanted considered on the proposed components were not presented in robust summary format as required under the HPV Challenge Program, and the

[4] Class 2 denotes a chemical that occurs as a complex mixture of different individual substances rather than existing as a single chemical species with a well-defined molecular structure (e.g., a paraffin wax). Class 2 compounds also include unknown or variable composition complex reaction products, biological materials (UVCB). UVCB substances can for example be described by structural features (e.g. acid chlorides, alkaline earth compounds, polyoxyalkylenes), a significant precursor (e.g. Castor Oil or Tallow) or by a more general description (e.g. Resins or Waxes).

quality/reliability of the suggested information was not presented; (3) The level of detail was inadequate to allow an independent assessment of study adequacy; and (4) the chemical di-2-ethylhexyl ether (CASRN 10143-60-9), which the sponsor states may make up 25 - 35 percent of the mixture known as Solvent C has information for only one SIDS endpoint, acute toxicity. More critically, the revised test plan did not provide a clear strategy for how data for individual components of Solvent C could be used to characterize the properties of the mixture, as acknowledged by the statement (p. 6 of the revised test plan) "it is unknown as to how the toxicity of the chemicals comprising it may change due to their presence as a mixture". Because of the uncertainties involved in using data for the components of Solvent C to characterize the toxicity of the mixture, only data for the sponsored substance, CASRN 68990-21-6 (aldehydes, C4, self-condensation products, high-boiling fraction), were considered in assessing the adequacy of human health effects and aquatic toxicity endpoints in this hazard characterization.

1. Chemical Identity

1.1 Identification and Purity

The following description is taken from the 2003 Test Plan.

Solvent C is a yellow-green liquid Class 2 chemical by-product from the combination of waste streams from four different processes used in the manufacture of other chemicals. [Note: These processes were not identified by the sponsor.] The sponsor stated that Solvent C may consist of many different chemicals with approximately 10 major constituents whose presence, and percentage, is dictated by the contributing waste stream. Since each waste stream contributes a different set of components to Solvent C, the presence or absence of any particular waste stream will significantly alter the composition of Solvent C.

1.2 Physical-Chemical Properties

The physical-chemical properties of CASRN 68990-21-6 could not be determined because no data are available

2. General Information on Exposure

2.1 Production Volume and Use Pattern

CASRN 68990-21-6 had an aggregated production and/or import volume in the United States between one million pounds and ten million pounds during calendar year 2005.

Non-confidential information in the IUR indicated that the industrial processing and uses for the chemical include other basic organic chemical manufacturing as solvents (for chemical manufacture and processing and are not part of product at greater than 1% by weight.) No commercial and consumer uses were reported for this chemical.

2.2 Environmental Exposure and Fate

The environmental fate properties of CASRN 68990-21-6 could not be determined because no data are available

3. Human Health Hazard

No human health toxicity data were submitted for SIDS endpoints for CASRN 68990-21-6; therefore, data gaps are listed for all SIDS endpoints in Table 3.

Acute, Repeated-Dose, Reproductive, Developmental, and Genetic Toxicity

No data were provided on CASRN 68990-21-6.

Conclusion: The potential health hazard of CASRN 68990-21-6 cannot be evaluated because no data are available.

Table 3. Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program – Human Health Data

Endpoints	SPONSORED CHEMICAL Aldehydes, C4, Self-Condensation Products, High-Boiling Fraction (68990-21-6)
Acute Toxicity LD_{50} (mg/kg)/LC_{50}	**No data**
Repeated-Dose Toxicity NOAEL/LOAEL	**No data**
Reproductive Toxicity NOAEL/LOAEL	**No data**
Developmental Toxicity NOAEL/LOAEL Maternal/Developmental Toxicity	**No data**
Genetic Toxicity – Gene Mutation	**No data**
Genetic Toxicity – Chromosomal Aberrations	**No data**

4. Hazard to the Environment

No aquatic toxicity data were submitted for SIDS endpoints for CASRN 68990-21-6; therefore, data gaps are listed for all SIDS endpoints in Table 4.

Acute Toxicity to Fish and Aquatic Invertebrates and Toxicity to Aquatic Plants

No data were provided on CASRN 68990-21-6.

Conclusion: The potential aquatic toxicity of CASRN 68990-21-6 cannot be evaluated because no data are available.

Table 4. Summary Table of the Screening Information Data Set as Submitted under the U.S. HPV Challenge Program - Aquatic Toxicity Data

Endpoint	SPONSORED CHEMICAL Aldehydes, C4, Self-Condensation Products, High-Boiling Fraction (68990-21-6)
Fish **96-h LC_{50} (mg/L)**	**No data**
Aquatic Invertebrates **48-h EC_{50} (mg/L)**	**No data**
Aquatic Plants **72-h EC_{50} (mg/L)** **(biomass)** **(growth rate)**	**No data**