Supporting Documents for Initial Risk-Based Prioritization of High Production Volume Chemicals

Chemical/Category: **Hexabromocyclododecane (HBCD)**
CAS 3194-55-6 1,2,5,6,9,10 hexabromocyclododecane
CAS 25637-99-4 hexabromocyclododecane

Contents:

QUALITATIVE SCREENING-LEVEL RISK CHARACTERIZATION FOR Hexabromocyclododecane (CAS No. 3194-55-6)

1. Background

The High Production Volume (HPV) Challenge Program[1] is 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 (U.S.) in quantities greater than one million pounds per year. In the Challenge Program, producers and importers of HPV chemicals voluntarily sponsor chemicals; sponsorship entails the identification and initial assessment of the adequacy of existing toxicity data/information, conducting new testing if adequate data do 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[Error! Bookmark not defined.,2]) endpoints that are screening-level indicators of potential hazards (toxicity) for humans or the environment and environmental fate.

The Environmental Protection Agency's Office of Pollution Prevention and Toxics (OPPT) is evaluating the data submitted in the HPV Challenge Program on approximately 1,400 sponsored chemicals. Data submitted to the Organisation for Economic Co-operation and Development (OECD) HPV Programme are also being evaluated. OPPT developed a screening-level hazard characterization that consists of an objective evaluation, conducted according to established EPA guidance**Error! Bookmark not defined.**[,3], of the quality and completeness of the data set provided and is based primarily on hazard data provided by sponsors. The characterization does not draw conclusions regarding the completeness of all data generated with respect to a specific chemical substance or mixture. The OECD SIDS documents (SIDS Initial Assessment Profile; SIAP and SIDS Initial Assessment Report; SIAR) provide similar information. Under both the HPV Challenge and OECD HPV Programs, chemicals that have similar chemical structures, properties and biological activities may be grouped together and their data shared across the resulting category. Evaluation of chemical category formation and data extrapolation(s) among category members is performed in accord with established U.S. EPA[1] and OECD[4] guidance.

In 2006 and 2007, EPA received data on uses of and reasonably likely exposures to chemicals on the Toxic Substances Control Act (TSCA) Inventory of existing chemicals, submitted in accordance with the requirements of the Inventory Update Reporting (IUR) rule[5]. Information is collected every five years under IUR, promulgated under the authority of section 8(a) of TSCA. The most recent reports pertain to chemicals manufactured in (including imported into) the U.S. during calendar year 2005 in quantities of 25,000 pounds or more at a single site. Information is reported on the identity of the chemical manufactured or imported and the quantity, physical form, and number of persons reasonably likely to be exposed during manufacture of the chemical. For chemicals manufactured or imported in quantities of 300,000 pounds or more at a single site during calendar year 2005, additional information was reported on the industrial processing and uses of the chemical, the number of industrial processing sites and of employees reasonably likely to be exposed to the chemical at these sites, the consumer and commercial uses of the chemical and an indication whether the chemical is used in products intended for use by children under 14 years of age.

For these qualitative screening-level risk characterization documents, EPA has reviewed the IUR data to evaluate exposure potential. In addition, exposure information that may have become available through prior Agency actions has been considered, as appropriate. The resulting exposure information has been combined with the screening-level hazard characterizations to develop this qualitative screening-level risk characterization[6,7]. These screening-level risk characterizations are technical documents intended to support subsequent decisions and actions by OPPT. Accordingly, the document is not written with the goal of informing the general public. The purpose of the

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[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.
[4] OECD. Guidance Document on the Development and Use of Chemical Categories; http://www.oecd.org/document/7/0,2340,en_2649_34379_1947463_1_1_1_1,00.html.
[5] U.S. EPA – Basic IUR Information: http://www.epa.gov/opptintr/iur/pubs/guidance/basic-information.htm
[6] U.S. EPA Guidelines for Exposure Assessment; http://cfpub.epa.gov/ncea/raf/recordisplay.cfm?deid=15263
[7] U.S. EPA. Risk Characterization Program; http://www.epa.gov/osa/spc/2riskchr.htm.

qualitative screening level risk characterizations is two-fold: to support initial risk-based decisions to prioritize chemicals and inform risk management options and to identify data needs for individual chemicals or chemical categories.

2. Physical-Chemical Properties and Environmental Fate

This report was prepared using the best available data from a number of sources, but draws no conclusions regarding whether additional relevant data may exist. 1,2,5,6,9,10-Hexabromocyclododecane (hexabromocyclododecane or HBCD) is a solid at room temperature. It has low water solubility, low vapor pressure, and moderate volatility from water. It is not expected to hydrolyze but may photolyze slowly. It is minimally mobile in soil and water systems. Recent information (see Physical/Chemical and Environmental Fate Characterization supporting document for details) suggests that HBCD is relatively biodegradable at environmentally relevant concentrations. Thus, HBCD is considered bioaccumulative (B3) but not persistent (P1).

In addition, the physical-chemical properties of HBCD that allow it to exist in the atmosphere attached to small particles in air are likely to increase its resistance to degrade in the atmosphere, and thus enhance its potential for long-range transport. This may account for increasing levels of HBCD in biota at remote locations, as reported in recent publications (see note at end of Exposure Characterization below).

3. Hazard Characterization

This summary is based on information compiled both from the HPV Challenge Submission as well as the OECD SIDS Initial Assessment Profile (SIAP) which was presented at an OECD SIDS Initial Assessment Meeting (SIAM) in April, 2007 for HBCD. This document is presented in an international forum that involves review and endorsement by governmental authorities around the world. The U.S. EPA is an active participant in these meetings and accepts this process as a reliable screening-level hazard assessment for the purpose of the U.S. HPV Challenge qualitative risk characterization process. Thus, when such documents exist there is no need to generate a separate Hazard Characterization document. In this case, the SIDS Initial Assessment Report (SIAR) is a European Union risk assessment which is a substantial document that is well beyond the scope of this screening level hazard/risk characterization. The SIAP can be found at the following website: http://cs3-hq.oecd.org/scripts/hpv/ (click on search in the left hand column).

Aquatic Organism Toxicity: The available aquatic toxicity data for the HPV Challenge endpoints (the SIDS described above) with HBCD shows that the potential acute hazard for fish and aquatic invertebrates is low and the acute hazard for aquatic plants is high. Chronic aquatic toxicity testing shows the hazard concern is high in aquatic invertebrates. The overall concern for the environment is high based on acute aquatic toxicity to algae, chronic toxicity to invertebrates, and the high potential to bioaccumulate [see above].

Human Health Toxicity: The acute toxicity of HBCD is low via the oral, dermal and inhalation routes of exposure. HBCD has been shown to be mildly irritating to the eyes, not irritating to skin, and it is not considered a skin sensitizer. The potential toxicity from repeated oral exposure to HBCD was assessed in a variety of studies in laboratory animals. Liver effects were observed in several studies but based on the inconsistency of effects between studies and sexes, and lack of dose-response, it is not clear if the observed effects are treatment-related. Effects on the thyroid (one or both sexes) were observed at moderate to high doses in some repeated-dose studies but not others, but could be due to the fact that the thyroid system was not thoroughly studied in the early studies. More recent studies showed increased thyroid weights in females only. One study indicates decreased serum T4 and increased serum TSH in both sexes, whereas another study only shows effects in females. Taken together, however, the data are suggestive of possible treatment-related thyroid effects in adult animals. Several recent *in vivo* and *in vitro* studies have been conducted to try and elucidate the possible mechanisms for both the observed liver and thyroid effects, but with no clear conclusions. Functional observation battery and motor activity evaluations in adult animals showed no evidence of neurotoxicity. The reproductive toxicity of HBCD was not specifically tested (i.e., there were no studies on fertility); however, repeated dose studies included an investigation of the reproductive organs. The only reproductive organ effects observed included transient increases in prostate weights at high doses (1,000 mg/kg/day); however, this occurred without any corresponding histopathology or functional changes in

several measured sperm parameters. Slight inhibition of oogenesis was also observed, but only at extremely high doses (>4 g/kg/day). Standard developmental toxicity studies with HBCD did not show any adverse effects on the developing fetus; however, disturbances in thyroid function observed in adult animals from repeated dose studies may have implications for the developing nervous system. The available data on genotoxicity shows that HBCD does not affect genes or chromosomes in various tests with bacteria, cell cultures, and whole animal tests.

HBCD was considered a candidate for further work in the OECD SIDS Programme based on repeated dose toxicity and possible developmental neurotoxicity (the latter based on a test that is beyond the SIDS). For the purposes of the U.S. HPV Challenge Program and this qualitative risk screening process, the overall human health hazard concern is moderate based on data suggestive of thyroid effects which could potentially affect developing fetuses in pregnant animals.

4. Exposure Characterization

This exposure characterization was completed using available 2006 Inventory Update Rule (IUR) submissions. Data and information that are claimed Confidential Business Information (CBI) by the submitter were reviewed and considered by EPA in preparing this assessment but are not disclosed in this summary.

In addition, the following sources were reviewed to identify exposure and use information: the HPV Challenge Submission, the OECD HPV Submission, the Toxics Release Inventory (TRI)**,** OSHA PEL documentation, various databases and public sources. See the separate Exposure Characterization for references.

HBCD was manufactured in the United States in amounts ranging from 10,000,000 to 50,000,000 pounds in 2005. The HPV submission indicates that HBCD's reported use is as a flame retardant. Its primary application is in extruded and expanded polystyrene foam that is used as thermal insulation in the building industry. A secondary application is as a flame retardant for upholstery textiles. A minor application is in video or audio equipment housing. In addition, other public sources report that HBCD is also used in crystal and high-impact polystyrene, SAN (styrene-acrylonitrile) resins, adhesives and coatings.

Exposures to Workers
A search of the National Occupational Exposure Survey (NOES), conducted from 1981 to 1983, has no data for the total number of workers potentially exposed to HBCD under the CAS No. 3194-55-6 but, the NOES estimated a total of 11,921 workers potentially exposed to this chemical under CAS No. 25637-99-4. Based on IUR reporting, which included at least one report that worker information was not readily obtainable, the maximum total number of workers likely to be exposed to this chemical during manufacturing and industrial processing and use is between 100 and 999. There may be additional potentially exposed workers that are not included in this estimate since not all production volume has been accounted, and there is at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions. HBCD has a vapor pressure of 4.70E-5 torr at 21°C. OPPT has established 0.001 torr as a value above which worker exposures to vapors should be estimated for chemical assessments. Below this value, OPPT assumes exposure to vapor is negligible. However, exposures may occur through inhalation of dusts and dermal contact. HBCD does not have an OSHA Permissible Exposure Limit.

Based on IUR data, specifically the number of potentially exposed workers and use codes, the potential worker exposure is high.

Exposures to the General Population and the Environment
HBCD is not on the Toxic Release Inventory. As an additive flame retardant, HBCD is not chemically bound to the matrix of the material it protects and thus has the potential to enter the environment. Based on this use information, EPA assumes for the purpose of this risk prioritization that there is potential for exposures to the general population and the environment.

The IUR-based ranking for general population and the environment is high due to the assumption that there will be exposure to this chemical.

In addition, public sources (see Exposure Characterization) report that HBCD's production and use as an additive flame retardant for extruded and expanded polystyrene foam, as well as uses in resins, adhesives, and coatings, may result in releases to the environment through various waste streams.

Exposures to Commercial Workers and Consumers
The IUR information has some commercial/ consumer products listed for HBCD (fabrics, textiles, apparel, rubber and plastics). Depending on the product, commercial workers and consumers may have potential dermal and inhalation exposure to the chemical.

The IUR-based ranking for commercial workers/consumers is high due to the assumption that HBCD is used in consumer/commercial products.

Exposures to Children
The IUR information suggests either that HBCD will not be used in children's consumer products or that this type of information is not readily available. Therefore, because of this uncertainty, the IUR-based ranking for children is moderate due to the assumption that HBCD may be present in products intended to be used by children.

NOTE: Although not discussed in the Exposure Characterization, for the purposes of this risk characterization, the Agency acknowledges the existence of recent reports in the scientific literature regarding the detection of HBCD in indoor air samples in homes around the world (*Environmental Science and Technology, 2008, Volume 42, pp. 459-464*). Also, environmental monitoring data show the presence of HBCD in freshwater (fish, invertebrates, plants), marine (porpoise, seal, and eel), and avian (hawks and falcons) organisms (as reported in both the OECD SIDS SIAP and the HPV Challenge Submission). However, OPPT has not fully evaluated any of this information for this risk characterization.

5. Risk Characterization

The statements and rationale provided below are intended solely for the purpose of this screening-level and qualitative risk characterization and will be used for prioritizing substances for future work in the U.S. HPV Challenge Program.

5.1. Risk Statement and Rationale

Potential Risk to Aquatic Organisms from Environmental Releases (HIGH CONCERN): EPA assumes there is potential for exposure to aquatic organisms from environmental releases. The bioaccumulation potential and high hazard for HBCD under acute (aquatic plants) and chronic (aquatic invertebrates) conditions suggest a high concern for potential risk to aquatic organisms from environmental releases, although the low persistence may mitigate this to some degree.

Potential Risk to the General Population from Environmental Releases (MEDIUM CONCERN): EPA assumes there is potential for exposure to the general population from environmental releases. The moderate concern for hazard to human health combined with the potential environmental exposures and low persistence suggests a medium concern for potential risk to the general population from environmental releases.

Potential Risk to Workers (HIGH CONCERN): Data suggest that workers may be exposed to HBCD. The moderate concern for hazard to human health combined with the likely exposures that occur in the occupational setting suggests a high concern for potential risk to workers.

Potential Risk to Commercial Workers and Consumers from Known Uses (HIGH CONCERN): IUR information suggests that commercial workers and consumers may be exposed to HBCD. Recent findings in the scientific literature also suggest the potential for consumer exposures from HBCD use, although this requires further evaluation. The moderate concern for hazard to human health combined with the likely exposures that occur in commercial worker/consumer use settings suggests a high concern for potential risk to commercial workers and consumers.

Potential Risk to Children (HIGH CONCERN): Information suggests that HBCD will be used in consumer products. It is likely that children will be exposed to consumer products containing this chemical. The moderate concern for hazard to human health is important in the case of children's health because studies have indicated that changes in thyroid function may lead to abnormal development, particularly for the developing nervous system. Therefore, the overall moderate human health hazard concern (and specific concerns for developmental effects) combined with expected exposures suggests a high concern for potential risks to children.

5.2. Uncertainties

HBCD may have minor uses that were not reported in IUR. In addition, there is uncertainty regarding the significance of the thyroid effects and the suggested potential for possible developmental neurotoxicity effects. Finally, although reproductive organ effects were seen only at high doses in a repeated dose study, the lack of a reproductive toxicity introduces some additional uncertainty.

5.3. Data Needs

The potential data need concerning developmental neurotoxicity from thyroid effects in pregnant animals is expected to be identified and addressed in the upcoming Integrated Risk Information System (IRIS) evaluation of HBCD (initiated in 2008 see http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=187215). IRIS assessments address the adequacy of data and the quality of existing studies, which are factors beyond the scope of this screening-level prioritization exercise.

Exposure Characterization for HPV Challenge Chemical

1,2,5,6,9,10 – Hexabromocyclododecane

CAS # 3194-55-6 and 25637-99-4

March 14, 2008

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Exposure Characterization for HPV Challenge Chemical

1,2,5,6,9,10 – Hexabromocyclododecane (CAS #3194-55-6 and 25637-99-4)

Non-CBI Executive Summary

Hexabromocyclododecane (HBCD) has a production volume in the range of >10 million - 50 million pounds (USEPA, 2006). Persons submitting Inventory Update Reporting (IUR) information in 2006 asserted that some of the information was confidential and therefore cannot be disclosed. Data and information that are CBI have been excluded from this summary.

Data provided in the HPV submission indicate that HBCD is used solely as a flame retardant. Its primary application is in extruded (XPS) and expanded (EPS) polystyrene foam that is used as thermal insulation in the building industry. A secondary, though important, application of HBCD is as a flame retardant for upholstery textiles. A minor application for HBCD is in video or audio equipment housings (BFRIP, 2005).

Recent studies show that HBCD is degraded in aquatic sediment and soil under aerobic and anaerobic conditions by a combination of abiotic and biotic processes, with half-lives of 2 days to 2 months. Therefore, it is rated as not persistent (i.e. P1). However, a BCF value of 18,100 indicates that 1,2,5,6,9,10-HBCD is highly bioaccumulative (B3) (USEPA, 2007b).

Exposure was characterized using both public, non-confidential sources and one or more IUR submissions available at the time the exposure characterization was written. If additional information warrants an update of the exposure characterization, the update will be posted on the EPA website.

A SIDS dossier has been prepared for this chemical.

Exposures to Workers

This chemical has a vapor pressure of 4.70E-5 torr at 21°C (USEPA, 2007b). OPPT has established 0.001 torr as a value above which worker exposures to vapors should be estimated for chemical assessments. Below this value, OPPT assumes exposure to vapor is negligible. Based on IUR data, some of which may contain CBI, other types of worker exposures are possible for this chemical. In fact, the Hazardous Substance Data Bank states that: "Occupational exposure to 1,2,5,6,9,10-hexabromocyclododecane may occur through inhalation of dusts and dermal contact with this compound at workplaces where 1,2,5,6,9,10-hexabromocyclododecane is produced or used" (HSDB, 2008). HBCD does not have an OSHA Permissible Exposure Limit (NIOSH, 2007a).

The National Occupational Exposure Survey (NOES), conducted from 1981 to 1983, has no data for the total number of workers potentially exposed to HBCD under the CAS number 3194-55-6 (NIOSH, 2007b) but, the NOES estimated a total of 11,921 workers potentially exposed to this

chemical under CAS number 25637-99-4 (NIOSH, 2007c). Based on IUR reporting, the maximum total number of workers likely to be exposed to this chemical during manufacturing and industrial processing and use is between 100 and 999. There may be additional potentially exposed workers that are not included in this estimate since not all production volume has been accounted, and there is at least one use that contains a "Not Readily Obtainable" (NRO) response among the submissions. This estimate does not include potentially exposed commercial workers.

Differences between numbers of workers estimated by IUR submitters and by the NOES are attributable to many factors, including time, scope, and method of the estimates. For example, NOES estimates are for all workplaces while IUR are for industrial workplaces only, and NOES used a survey and extrapolation method while IUR submitters simply provide their best estimates based on available information for the specific reporting year.

Based on IUR data, specifically the number of potentially exposed workers and use codes, the potential worker exposure is considered high.

Exposures to the General Population and the Environment

HBCD is not on the Toxics Release Inventory (USEPA, 2007a) and no direct information from the other sources that were searched is available on environmental releases. Additionally, HBCD's production and use as an additive flame retardant for extruded and expanded polystyrene foam, as well as crystal and high-impact polystyrene, SAN (Styrene-AcryloNitrile) resins, adhesives, and coatings, may result in releases to the environment through various waste streams because, as an additive flame retardant, it is not incorporated into the matrix of the material it protects and so has the potential to enter the environment (HSDB, 2008). Based on the totality of the information and expert judgment, EPA assumes, for the purpose of this risk based prioritization, that the potential for exposures to the general population and the environment is high.

Exposures to Commercial Workers and Consumers

IUR information has some commercial/consumer products listed, such as, fabrics, textiles, apparel, rubber and plastics. Depending on the product, commercial workers and consumers may have potential exposure to the chemical. The likelihood that this chemical is used in consumer/commercial products is high based on IUR data.

Exposures to Children

Information suggests either that HBCD will not be used in children’s consumer products or that this type of information is not readily available.

There is a moderate likelihood that this chemical is used in products intended to be used by children but there is uncertainty in the IUR data.

References

BFRIP, 2005. HPV Data Summary and Test Plan for Hexbromocyclododecane (HBCD). Original Submission: December 20, 2001 - Updated September 2003, March 2005. American Chemistry Council's Brominated Flame Retardant Industry Panel (BFRIP). Accessed January 2008 at http://www.epa.gov/chemrtk/pubs/summaries/cyclodod/c13459rt.pdf

HPVIS, 2007. U.S. EPA. High Production Volume Information System. http://www.epa.gov/hpv/hpvis/index.html.

HSDB,2008. Hazardous Substances Data Bank. As cited in HSDB record for Hexabromocyclododecane, CAS 3194-55-6, accessed January 7, 2008. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB.

NIOSH, 2007a OSHA PEL Project Documentation. Accessed August, 2007. http://www.cdc.gov/niosh/pel88/npelcas.html.

NIOSH, 2007b. National Occupational Exposure Survey (Survey for 1981-1983, NOES). Accessed December 2007. http://www.cdc.gov/search.do?action=search&subset=noes&queryText=3194-55-6&Go%21=Go%21

NIOSH, 2007c. National Occupational Exposure Survey (Survey for 1981-1983, NOES). Accessed December 2007. http://www.cdc.gov/noes/noes2/x2384occ.html

USEPA, 2006. 2006 Partial Updating of TSCA Chemical Inventory.

U.S. EPA, 2007a. Toxic Release Inventory. Accessed August, 2007. http://www.epa.gov/tri/.

USEPA 2007b. Physical/Chemical and Environmental Fate Characterization for High Production Volume Chemicals Chemical Name: Hexabromocyclododecane

PHYSICAL/CHEMICAL AND ENVIRONMENTAL FATE CHARACTERIZATION FOR HIGH PRODUCTION VOLUME CHEMICALS

CHEMICAL NAME:

1,2,5,6,9,10-HEXABROMOCYCLODODECANE (CAS NO. 3194-55-6)

FEBRUARY 12, 2008

Prepared by

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1. Executive Summary

This report was prepared using the best available data from a number of sources. 1,2,5,6,9,10-hexabromocyclododecane is a solid at room temperature. It has low water solubility, low vapor pressure, and moderate volatility from water. It is not expected to hydrolyze but may photolyze slowly. It is minimally mobile in soil and water systems. Recent information suggests that HBCD is relatively biodegradable at environmentally relevant concentrations. Thus, HBCD is considered highly bioaccumulative (B3) but not persistent (P1). In addition, the predicted atmospheric oxidation half-life for HBCD meets the long-range transport criterion (half-life in air of 2 days) of the UNECE-LRTAP and UNEP conventions.

2. Fate Characterization Summary for 1,2,5,6,9,10-Hexabromocyclododecane

The following summary of the fate of 1,2,5,6,9,10-hexabromocyclododecane (HBCD) is derived from information contained within the Hazardous Substance Data Bank (HSDB, 2007), High Production Volume Test Plans (ACC, 2002), EPISuite™ (USEPA, 2007b), and recent publications by Davis et al. (2005; 2006).

As cited in HSDB (2007), 1,2,5,6,9,10-HBCD production and use as an additive flame retardant may result in its release to the environment through various waste streams. If released to air, a vapor pressure of $4.7x10^{-7}$ mm Hg at 21° C indicates 1,2,5,6,9,10-HBCD will exist in both the vapor and particulate phases. Vapor-phase 1,2,5,6,9,10-HBCD will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 1-3 days. Particulate-phase 1,2,5,6,9,10-HBCD will be removed from the atmosphere by wet and dry deposition. If released to soil, 1,2,5,6,9,10-HBCD is expected to be minimally mobile based upon an estimated K_{oc} values of 60,000 to 125,000. Volatilization from moist soil surfaces may be an important fate process based upon an estimated Henry's Law constant of $4.6x10^{-5}$ atm-m^3/mole; however, adsorption to soil is expected to greatly attenuate volatilization. 1,2,5,6,9,10-HBCD is not expected to volatilize from dry soil surfaces based upon its low vapor pressure. If released into water, 1,2,5,6,9,10-HBCD is expected to adsorb to suspended solids and sediment based upon the estimated K_{oc}. Volatilization from water surfaces may be an important fate process based upon this compound's estimated Henry's Law constant; however, adsorption is expected to severely attenuate volatilization. A BCF of 18,100, was measured in fathead minnows exposed to 6.2 μg/L of 1,2,5,6,9,10-HBCD over the course of a 32-day incubation period. According to a classification scheme, this BCF suggests the potential for bioconcentration in aquatic organisms is high.

3. Disposition in Land, Water, Air

Terrestrial Fate (as cited in HSDB, 2007a, EPA 2007a)
Based on a classification scheme, estimated K_{oc} values in the range of 60,000 to 125,000 indicates that 1,2,5,6,9,10-HBCD is expected to be minimally mobile in soil. Volatilization of 1,2,5,6,9,10-HBCD from moist soil surfaces may be an important fate process given an estimated Henry's Law constant of $4.6x10^{-5}$ atm-m^3/mole derived from its vapor pressure, $4.7x10^{-7}$ mm Hg at 21° C, and water solubility of 8.6 μg/L. However, adsorption to soil is expected to attenuate volatilization. 1,2,5,6,9,10-HBCD is not expected to volatilize from dry soil surfaces based upon

its estimated vapor pressure. 1,2,5,6,9,10-HBCD achieved 0% of its theoretical BOD in a Closed Bottle aerobic biodegradation test over a 28 day incubation period. Based upon these results, biodegradation of 1,2,5,6,9,10-HBCD is classified as not readily biodegradable. However, recent work (Davis et al. 2005, 2006) suggests that it is relatively biodegradable at environmentally relevant concentrations. This work showed that HBCD was degraded in soil and aquatic sediment under aerobic and anaerobic conditions by a combination of abiotic and biotic processes, with half-lives of 2 days to 2 months.

Aquatic Fate (as cited in HSDB, 2007a, EPA 2007a)

Based on a classification scheme, estimated K_{oc} values of 60,000 to 125,000, indicate that 1,2,5,6,9,10-HBCD is expected to adsorb to suspended solids and sediment. Volatilization from water surfaces may occur based upon a estimated Henry's Law constant of $4.6x10^{-5}$ atm-m^3/mole derived from its vapor pressure, $4.7x10^{-7}$ mm Hg at 21° C, and water solubility of 8.6 µg/L; however, adsorption is expected to attenuate volatilization. A BCF of 18,100, measured in fathead minnows, suggests the potential for bioconcentration in aquatic organisms is high. In addition, recent work (Davis et al. 2005, 2006) suggests that it is relatively biodegradable at environmentally relevant concentrations. This work showed that HBCD was degraded in aquatic sediment and soil under aerobic and anaerobic conditions by a combination of abiotic and biotic processes, with half-lives of 2 days to 2 months.

Atmospheric Fate (as cited in HSDB, 2007a, EPA 2007a)

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere, 1,2,5,6,9,10-HBCD, which has a vapor pressure of $4.7x10^{-7}$ mm Hg at 21° C, is expected to exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase 1,2,5,6,9,10-HBCD is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 1-3 days Particulate-phase 1,2,5,6,9,10-HBCD may be removed from the air by wet and dry deposition. Sorption to the atmospheric particulate phase may increase resistance of atmospheric HBCD to oxidation, and thus enhance its potential for long-range transport.

4. Persistence and Bioaccumulation

Persistence and bioaccumulation are qualitatively characterized according to the criteria set forth in the PMN program (FR, 1999). Recent studies show that HBCD is degraded in aquatic sediment and soil under aerobic and anaerobic conditions by a combination of abiotic and biotic processes, with half-lives of 2 days to 2 months. Therefore, it is rated as not persistent (i.e. P1). However, a BCF value of 18,100 indicates that 1,2,5,6,9,10-HBCD is highly bioaccumulative (B3).

5. Data Gaps

No data gaps were identified.

6. Summary of Physical Chemical Properties

Figure 1 shows the structure of 1,2,5,6,9,10-HBCD. Basic physical-chemical properties of 1,2,5,6,9,10-HBCD are presented in Table 1, and environmental fate properties are given in Table 2. The persistence-bioaccumulation rankings are given in Table 3, showing a ranking of P1B3 for 1,2,5,6,9,10-HBCD.

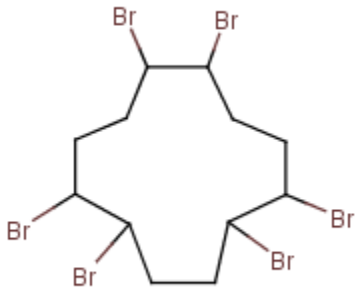

Figure 1. Structure of 1,2,5,6,9,10-Hexabromocyclododecane (USEPA, 2007b)

Table 1. Physical-Chemical Properties of 1,2,5,6,9,10-Hexabromocyclododecane.		
Property	Value/Quality	References
CAS No.	3194-55-6	
IUPAC	1,2,5,6,9,10-HBCD	
Molecular Weight	631.69	ACC (2002)
Physical State	Solid	ACC (2002)
Melting Point	175–190° C[a]	ACC (2002)
Boiling Point	462° C (estimated); 230 °C (decomposes)	ACC (2002)
Vapor Pressure	4.7×10^{-7} mm Hg at 21° C (measured)	ACC (2002)
Water Solubility	3.4 µg/L at 25° C (measured) 8.6 µg/L at 25° C (measured)	ACC (2002) HSDB 2007
Density	No data	
Log K_{ow}	5.625 at 25° C (measured)	ACC (2002)
[a] Range of melting points provided by the commercial manufacturers.		

Table 2. Environmental Fate Properties of 1,2,5,6,9,10-Hexabromocyclododecane.		
Property	Value/Quality	References
Photodegradation	Half-life = 25.6 hours (calculated) Half-life = 3 days (calculated)	ACC (2002) HSDB 2007
Aerobic Degradation	No biodegradation observed (closed-bottle test over a 28-day incubation period at 18–20° C) Half-lives for aquatic sediment = 11-32 days; soil = 63 days	ACC (2002) Davis et al. (2005, 2006)
Anaerobic Degradation	Half-lives for aquatic sediment = 1.1-1.5 days; soil = 6.9 days	Davis et al. (2005, 2006)
Hydrolysis	$1.8x10^{5}$ years pH 8 (calculated) $1.8x10^{6}$ years pH 7 (calculated)	ACC (2002)
Bioaccumulation	BCF = 18,100 measured in fathead minnows	HSDB 2007
Henry's Law Constant	$6.4x10^{-11}$ atm-m^3/mole at 25° C (estimated) $4.6x10^{-5}$ atm-m^3/mole (estimated)	ACC (2002) HSDB 2007
Direct photolysis	Not significant	ACC (2002)
K_{oc}	$1.25x10^{+5}$ mL/g (estimated) 60,000 mL/g (estimated)	ACC (2002) HSDB 2007
Fugacity	Air: 0.0007% Water: 2.1% Soil: 40% Sediment: 58%	USEPA (2007) [a] ACC (2002)
[a] The model was run using the default values of the EPI Suite Level III (USEPA, 2007b).		

Table 3. Persistence and Bioaccumulation of 1,2,5,6,9,10-Hexabromocyclododecane.		
Property	Value/Quality	References
Persistence	P1 (high)	FR (1999)
Bioaccumulation	B3 (high)	FR (1999)

6. References

ACC, 2002. Robust Summaries & Test Plans: Cyclododecane. HPV Test Plan. Submitted by American Chemistry Council (ACC) Brominated Flame Retardant Industry Panel (BFRIP). U.S. Environmental Protection Agency: Washington, DC. Accessed August 23, 2007. http://www.epa.gov/chemrtk/pubs/summaries/cyclodod/c13459tc.htm.

Davis JW, S Gonsior, G Marty, J Ariano. 2005. The transformation of hexabromocyclododecane in aerobic and anaerobic soils and aquatic sediments. Water Res. 39:1075-1084.

Davis JW, SJ Gonsior, DA Markham, URS Friederich, RW Hunziker, JM Ariano. 2006. Biodegradation and product identification of [^{14}C]hexabromocyclododecane in wastewater sludge and freshwater sediment. Environ. Sci. Technol. 40:5395-5401.

FR 1999, Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances. *Federal Register* 64, Number 213 (November 4, 1999) Page 60194-60204

HSDB. 2007. Hazard Substances Data Base. As cited in HSDB record for 1,2,5,6,9,10-Hexabromocyclododecane. Accessed August 23, 2007. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB.

USEPA. 2007. EPI Suite v3.2 PC-Computer software developed by the EPA Office of Pollution Prevention Toxics and Syracuse Research Corporation. http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.