B14-1.0 HEXACHLOROACETONE (HCA)

B14-1.1 Background Information

IUPAC: Hexachloroacetone; Perchloroacetone

CAS: 1,1,1,3,3,3-hexachloro-2-propanone

CASRN: 116-16-5

HEXACHLOROACETONE USES:

HCA was used as a pre and post-emergence herbicide. However, it no longer has any commercial use as an herbicide. A former use of HCA was as a pre-harvest desiccant on alfalfa seed crops (HSDB, 2003).

HCA was used in conjunction with 2,4,5-T, and it was only applied during the 1967 U.S. trials (Demaree and Haws, 1968).

Table B14-1 HCA Usage at CFB Gagetown[a]

Year	Amount of HCA Applied (kg)	Total Area Treated (ha)
1967	16.3	2.4
Total	**1.6E+01**	**2.4E+00**

[a] Adapted from Demaree and Haws, 1968.

B14-1.0 CHEMICAL AND PHYSICAL PROPERTIES

Formula: C_3Cl_6O

Activity: Halogenated aliphatic herbicides

Notes: HCA is not registered as an herbicide in Canada or the United States (PAN, 2006). Limited information exists regarding the toxicology of HCA as an herbicide. All information that had been found was presented below. Databases searched include: U.S. EPA, IRIS database, RED database, IPCS INCHEM database, ATSDR CDC database, WHO, UNEP, PUBMED, EMBASE, NTP, Google keyword search, and PAN pesticide databases.

Structure:

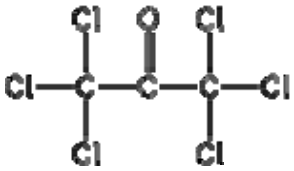

Figure B14-1 HCA CASRN: 116-16-5 Structure

Table B14-2 Chemical and Physical Properties of HCA

Chemical/Physical Property	Result	Reference
Colour/form	Very light yellow liquid	HSDB, 2003
Odour	Musty odour	HSDB, 2003
Henry's Law constant	$9.47x10^{-8}$atm-m^3/mole at 25ºC	JW, 2006
Log K_{ow}	2.48-3.69	JW, 2006
Molecular Weight	264.75	JW, 2006
Vapour Pressure	0.123mm Hg at 25ºC	JW, 2006
Solubility	150mg/L at 25ºC	JW, 2006
K_{oc}	1886	JW, 2006

B14-3.0 PMRA EVALUATION

No information found.

B14-4.0 TOXICOLOGICAL SUMMARY

B14-4.1 Human Health Effects

Table B14-3 Human Health Effects Resulting from Acute Exposure to HCA Containing Herbicides[a]

Exposure	Effects	Response
Acute	Dermal	Causes skin irritation, maybe be harmful if absorbed through the skin.
	Eye contact	Causes eye irritation.
	Respiratory	May be harmful if inhaled, may cause irritation to mucous membranes and upper respiratory tract.
	Hepatic	Liver is a target organ if ingested
	Genitourinary	Kidneys are target organs if ingested
	Nervous	May affect central nervous system if ingested

[a] Adapted from Sigma-Aldrich, 2006.

B14-4.2 Health Effects by Route of Exposure

B14-4.2.1 Oral Exposure

Table B14-4 Mammalian LD_{50} Values Resulting from Oral Exposure to Hexachloroacetone

Test Organism (Species/Sex)	LD_{50} (mg/kg)	Reference
Acute		
Rat	240	Sigma-Aldrich, 2006
Dog	700	Sigma-Aldrich, 2006

Table B14-5 Mammalian Reproductive and Developmental Effects Resulting from Oral Exposure to Hexachloroacetone

Test Organism (Species)	Exposure	Dose (mg/kg/day) (Duration)	Response	Reference
Rats	Drinking water	0, 25, 100, 400 ppm for 35 days	HCA may be taste-aversive at 400 ppm in male and female rats and is not a reproductive toxicant in males. HCA is a reproductive toxicant in females	NTP, 1997

B14-4.2.1.1 No Observed Adverse Effect Levels

No data found.

B14-4.2.2 Dermal Exposure

Table B14-6 Mammalian Acute LD_{50} Value Resulting from Dermal Exposure to Hexachloroacetone

Test Organism (Species/Sex)	LD_{50} (mg/kg)	Reference
Acute		
Rabbit	2,980	Sigma-Aldrich, 2006

B14-4.2.3 Inhalation Exposure

Table B14-7 Mammalian Acute LC_{50} Value Resulting from Inhalation Exposure to Hexachloroacetone

Test Organism (Species/Sex)	LC_{50} (mg/kg)	Reference
Acute		
Mouse	920 mg/m^3	Sigma-Aldrich, 2006
Rat	360 mg/m^3	Sigma-Aldrich, 2006

B14-4.3 Carcinogenicity

HCA was found to be mutagenic in the Ames strains TA98 and TA100 in the absence of solvents (26 mg HCA/plate). Mutagenic effects will be seen at lower dosage levels (1.75 mg HCA/plate) when dimethylsulfoxide was used as solvent for HCA. When DMSO solution of HCA was incubated above 20ºC, it developed a yellow colour and became more toxic to the test bacteria.

At this temperature, only 0.5 mg HCA/plate was needed to produce maximum number of revertants (Yamashita *et al*. 1987).

HCA was also an active mutagen in the E.coli strains WP-2 (tryptophan reversion assay) and in the rec-BC (recombination repair deficient) strains (Yamashita *et al*., 1987).

No other data were found about HCA's role in carcinogenesis.

B14-4.4 Populations at Special Risk

No data found.

B14-4.5 Toxicokinetics

No data found.

B14-4.6 Exposure Limits

Reference Dose (mg/kg/day)	Reference	Endpoint	Study	Reference	NOEL (mg/kg/day)	Uncertainty Factor
Acute/Short-term						
No information found	--	--	--	--	--	--
Intermediate- term						
No information found	--	--	--	--	--	--
Long-term						
0.001[a]	U.S. EPA, 1992	Atrophy and degeneration of the renal tubules	Rat Subchronic Dietary Study	Gorzinski *et al*., 1985	1.0	1,000

[a] Based on exposure limits for hexachloroethane.

For the risk assessment purposes, a long-term exposure limit of 0.001 was chosen for use.

B14-5.0 ENVIRONMENTAL FATE AND EXPOSURE

Air

HCA has a vapour pressure of 0.123 mm Hg at 25ºC (JW, 2006). Hence, if HCA is found in the atmosphere it will exist almost entirely in the vapour phase (HSDB, 2003). HCA is relatively inert in atmosphere and will not react with photochemically produced hydroxyl radicals (HSDB, 2003). No other data were found about HCA's chemical processes in air.

Water

When released in water, HCA will be expected to evaporate into the atmosphere with a volatilization half-life of 6.5 hours from a model river (HSDB, 2003). Having a K_{oc} of 1,886 (JW, 2006), HCA will be expected to partition from the water column to sediment (HSDB,

2003). No other data were found about HCA's chemical processes in water.

Sediment and Soil

HCA's K_{oc} value suggests that HCA will have low mobility in soil and have low likelihood to leach (HSDB). No other data were found about HCA's chemical processes in soil.

B14-6.0 SUMMARY

HCA was used as a pre/post-emergent selective herbicide (HSDB, 2003). However, it is no longer registered for use in Canada and the United States. During the 1967 U.S. trials, a small quantity of HCA was applied in a mixture with 2,4,5-T on selected test plots at CFB Gagetown (Demaree and Haws, 1968).

HCA has low acute toxicity. However, HCA induced reproductive effects in female rats during a NTP (1997) study. No other information regarding the toxicity of HCA was found.

B14-7.0 REFERENCES

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