

Triallyl Isocyanurate
[1025-15-6]

Review of Toxicological Literature

Prepared for

Errol Zeiger, Ph.D.
National Institute of Environmental Health Sciences
P.O. Box 12233
Research Triangle Park, North Carolina 27709
Contract No. N01-ES-65402

Submitted by

Raymond Tice, Ph.D.
Integrated Laboratory Systems, Inc.
P.O. Box 13501
Research Triangle Park, North Carolina 27709

July 1998

EXECUTIVE SUMMARY

Triallyl isocyanurate, a commonly used crosslinking agent, was nominated for evaluation by the National Institute of Environmental Health Sciences (NIEHS) due to its moderate volatility, which enhances the potential for exposure and the lack of toxicity data.

Conflicting physical and chemical characteristics are described in the literature for triallyl isocyanurate.

Triallyl isocyanurate may be produced by gradually adding cyanuric chloride to an excess of the allyl chloride or alcohol in the presence of concentrated aqueous base. Data on production and import volumes were not available.

Triallyl isocyanurate is used as a crosslinking agent in the manufacture of synthetic rubbers, flame retardants, and agrochemicals. The brominated form is marketed as a flame retardant for olefin and styrene resins, providing heat and weather resistance, good dispersability, and high heat stability (to prevent yellowing). Triallyl isocyanurate, polymerized with methacrylate and divinylbenzene, has been studied as an adsorbent for urea in artificial kidneys. Triallyl acetate has been utilized as a crosslinking agent in the synthesis of a chiral stationary phase for the resolution of amino acid enantiomers by high performance liquid chromatography (HPLC).

Trace amounts of triallyl isocyanurate have been detected in chemicals used in water treatment facilities. However, the principal concern with regard to human exposure to triallyl isocyanurate is the potential exposure to allyl alcohol and isocyanuric acid as products of thermal decomposition. A recent review of the toxicological literature on isocyanuric acid suggests that it has a low potential for human toxicity or carcinogenicity. The toxicity of allyl alcohol is currently being investigated.

No data were found on human toxicity related to triallyl isocyanurate.

Due to its use as a crosslinking agent in plastics used in food packaging, triallyl isocyanurate is regulated under section 21 of the Code of Federal Regulations (CFR) by the Food and Drug Administration (FDA) as an indirect food additive.

Based upon chemical structure, hydrolysis would be the most likely means of metabolism of triallyl isocyanurate, followed by elimination in the urine.

Acute toxicity data for triallyl isocyanurate consisted of an oral LD₅₀ study in rats, an ocular irritancy test in rabbits, and a skin irritation study in rabbits. The acute oral toxicity study indicates an LD₅₀ of approximately 1000 mg/kg (4.011 mmol/kg) in rats. Results of the dermal irritation study in rabbits indicate that a single, prolonged contact is essentially non-irritating. Results of the eye irritancy test in rabbits indicate that this material may produce light, transient conjunctival irritation. Results of a repeat dosing dermal irritation study in rabbits indicate that repeated contact may produce

slight redness and scaling. No data on the effect of chronic exposure were available for triallyl isocyanurate.

No data on the reproductive or teratological effects of triallyl isocyanurate were located.

No carcinogenicity data were located for triallyl isocyanurate.

Triallyl isocyanurate, in the absence and presence of metabolic activation, did not induce *his* gene mutations in *Salmonella typhimurium*, nor did it induce sister chromatid exchanges (SCE) in Chinese hamster ovary (CHO) cells. In *in vitro* clastogenicity studies with Chinese hamster lung (CHL) and CHO cells, triallyl isocyanurate induced chromosomal aberrations in the presence but not the absence of metabolic activation.

No data pertaining to the immunotoxicity of triallyl isocyanurate were available.

No information pertaining to the activity-structure relationships of triallyl isocyanurate was available.

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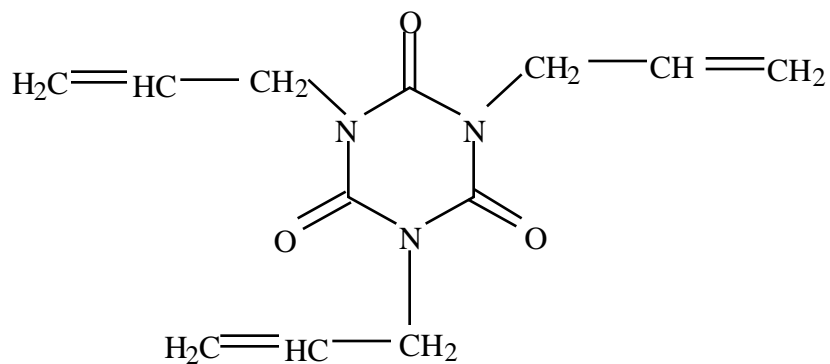
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1.0 BASIS FOR NOMINATION

Triallyl isocyanurate, a commonly used crosslinking agent, was nominated for toxicity and carcinogenicity testing by the National Institute of Environmental Health Services (NIEHS) because of its moderate volatility, which enhances the potential for exposure and the lack of toxicity data.

2.0 INTRODUCTION

Triallyl Isocyanurate
[1025-15-6]



2.1 Chemical Identification

Triallyl isocyanurate (C₁₂H₁₅N₃O₃; mol. wt. = 249.30) is also called:

1,3,5-Triallyl isocyanurate
s-Triazine-2,4,6(1*H*,3*H*,5*H*)-trione; 1,3,5-triallyl-
DIAK 7

Isocyanuric acid triallyl ester

TAIC

1,3,5-Triallylisocyanuric acid

Triallyl-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

1,3,5-Tri-2-propenyl-1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

Triallyl-s-triazine-2,4,6(1*H*,3*H*,5*H*)-trione

2.2 Physical-Chemical Properties

Property	Information	Reference
Physical Form	White, crystalline solid	Radian Corporation (1991)
Melting Point (°C)	23.5-25	Radian Corporation (1991)
Boiling Point (°C)	149.0-152.0 @ 4 mm Hg	Aldrich (1996-1997)
Flash Point (°C)	>110	Aldrich (1996-1997)
Density (°C, g/cm ³)	1.1159	Radian Corporation (1991)
Solubility (@ 20°C):		Radian Corporation (1991)
Water	<1 mg/mL	
DMSO	100 mg/mL	
95% Ethanol	100 mg/mL	
Acetone	100 mg/mL	
Refractive Index	1.5130	Aldrich (1996-1997)

The physical description and chemical characteristics as described by Dow (1977) are in conflict with those provided by the Radian Corporation (1991) and Aldrich (1996-1997). For example, Dow lists the physical description of triallyl isocyanurate as a clear liquid, while Radian lists a white, crystalline powder. A major discrepancy is also noted for the boiling point, listed as 302°C at 4 mm Hg by Dow and 149-152°C at 4 mm Hg by Radian. However, the CAS Registry Numbers provided in both sources are identical.

Compounds containing the allylic structure, such as triallyl isocyanurate, may form peroxides during storage when in contact with air (PTCL, 1998).

2.3 Commercial Availability

Triallyl isocyanurate is available commercially from the following sources in the United States (among others): Interbusiness Group, USA, Inc. (New York, NY); Monomer-Polymer & Dejac Labs, Inc. (Feasterville, PA); Nipa Hardwicke, Inc. (Wilmington, DE); Itochu Specialty Chemicals, Inc. (White Plains, NY); Azko-Nobel Chemicals, Inc. (Chicago, IL); and Aldrich Chemical Co. (Milwaukee, WI). It is also available from Nippon Kasai Chemical Company, Ltd. (Japan) (CW Buyer's Guide, 1998). The brominated form, known as Firecut-66 (Anon., 1986), is available from Suzuhiro Chemical (Japan).

3.0 PRODUCTION PROCESSES AND ANALYSES

No information on producers or production volumes was found in the Chemical Economics Handbook, PROMT database, or SRI Directory of Chemical Producers. Triallyl isocyanurate may be produced using either allyl chloride or allyl alcohol as the starting point (Anon., 1990), gradually adding cyanuric chloride to an excess of the allyl chloride or alcohol in the presence of concentrated aqueous base (Grayson, 1985). Triallyl isocyanurate is analyzed utilizing gas chromatography with nitrogen phosphorous detection (GC/NPD) (Ruth and Schill, 1968).

4.0 PRODUCTION AND IMPORT VOLUMES

Data on production and import volumes for triallyl isocyanurate were not available.

5.0 USES

Triallyl isocyanurate is used as a crosslinking agent in the manufacture of synthetic rubbers, flame retardants, and agrochemicals. The brominated form is marketed as a flame retardant for olefin and styrene resins (Anon., 1985). It provides heat and weather resistance, good dispersability, and high heat stability (to prevent yellowing) to the products to which it is added (Anon., 1978). Triallyl isocyanurate, polymerized with methacrylate and divinylbenzene, has been studied as an adsorbent for urea in artificial kidneys (Ho and Wu, 1987). Triallyl isocyanurate, polymerized with vinyl acetate, has been employed as a crosslinking agent in the synthesis of a chiral stationary phase for the resolution of amino acid enantiomers by high performance liquid chromatography (HPLC) (Ma, 1996).

6.0 ENVIRONMENTAL OCCURRENCE AND PERSISTENCE

Trace amounts of triallyl isocyanurate were detected in four different sources of liquid alum used in drinking water treatment facilities. Triallyl isocyanurate, in addition to other compounds, may be introduced into the water treatment chemicals during their manufacturing, packaging, or transportation (Thompson and Karasek, 1987).

7.0 HUMAN EXPOSURE

The principal concern with regard to human exposure to triallyl isocyanurate is the potential release of allyl alcohol during the formulation of some rubber compounds, since conditions conducive to ester decomposition may exist during this time (Drake et al., 1993). This is based upon the supposition that, like acrylic and methacrylic esters, which are known to release acrylic and methacrylic acid when heated, triallyl isocyanurate could release allyl alcohol and isocyanuric acid as products of thermal decomposition (Drake et al., 1993). A toxicological summary on isocyanuric acid, submitted to the National Toxicology Program (NTP) (June 1997) suggested that isocyanuric acid has a low potential for human toxicity or carcinogenicity. The toxicity of allyl alcohol is currently being examined by NTP (Report No. 48), scheduled for release in 1998.

8.0 REGULATORY STATUS

	Regulation	Effect of Regulation/Other Comments
F	21 CFR 177 Subpart C	Triallyl cyanurate appears in a table entitled, "Substances for Use Only as Components of Articles Intended for Repeated Use."
D	21 CFR 177 Part 177	Triallyl cyanurate appears in a list of chemicals under the section, 177.2420 Polyester Resins, cross-linked under Part 177 INDIRECT FOOD ADDITIVES: POLYMERS.
A	21 CFR 175 Subpart B	Triallyl cyanurate appears in a list of chemicals under the section, Substances for Use Only as Components of Adhesives under Part 175 INDIRECT FOOD ADDITIVES: ADHESIVES AND COMPONENTS OF COATINGS

9.0 TOXICOLOGICAL DATA

9.1 General Toxicology

9.1.1 Human Data

No data were found on human toxicity related to triallyl isocyanurate.

9.1.2 Chemical Disposition, Metabolism, and Toxicokinetics

No data on the disposition, metabolism, or toxicokinetics of triallyl isocyanurate were available. Based upon chemical structure, hydrolysis would be the most likely means of metabolism of triallyl isocyanurate (Parkinson, 1996), with elimination primarily in the urine (Rozman and Klaassen, 1996).

9.1.3 Acute Exposure

Acute exposure data for triallyl isocyanurate are presented in **Tables 1** and **2**.

The only acute toxicity data available were provided in a Dow Chemical Research and Development document (1977), which assessed the toxic potential of triallyl isocyanurate. The evaluation consisted of an oral LD₅₀ study in rats and an ocular irritancy test and skin irritation study in rabbits. These data were generated in 1977 and submitted to the U.S. Environmental Protection Agency (EPA) in 1992 as part of the Toxic Substances Control Act (TSCA) Section 8(e) Compliance Audit Program (CAP), which called for companies to submit to the EPA data on any chemical that might present a substantial risk to human health.

Table 1. LD₅₀ Value for Triallyl Isocyanurate

Route	Species (strain)	LD ₅₀ mg/kg(mmol/kg)	Reference
oral	rat (n.p.)	1000 (4.011)	Dow Chemical (1977)

Abbreviation: n.p. = not provided

Table 2. Acute Exposure to Triallyl Isocyanurate

Species, Strain, and Age	Number and Sex of Animals	Chemical Form, Purity	Dose	Exposure/Observation Period	Results/Comments	Reference
Rats						
Rat (strain, age n.p.)	3 M rats/dose Controls: None	Triallyl isocyanurate, purity n.p.	126, 252, 500, 1000, and 2000 mg/kg (0.505, 1.01, 2.01, 4.01, and 8.02 mmol/kg); p.o.	Single dose; observation period given as 14 d post-dose in methodology	Signs of toxicity included lethargy, listlessness, inability to walk, tremors, and red secretions around nares at 1000 and 2000 mg/kg.	Dow Chemical (1977)
Rabbits						
Rabbit (strain, age n.p.)	3 rabbits; 1 rabbit/ method Controls: None (sex n.p.)	Triallyl isocyanurate, purity n.p.	n.p. ¹ applied to (A) intact skin, (B) occluded skin, and (C) abraded skin	3 applications over 3 d, observation for 14 d (abraded skin)	No adverse effects observed.	Dow Chemical (1977)
Rabbit (strain, age n.p.)	1 rabbit Controls: None (sex n.p.)	Triallyl isocyanurate, purity n.p.	n.p.	Single application one eye rinsed, one eye not rinsed; observation for 24 h	Slight transient conjunctival irritation.	Dow Chemical (1977)

Abbreviations: n.p. = not provided; p.o. = *per os* = by mouth

¹Entry is not legible; possibly says "...applied as 15% solution in (diluent not provided)..." OR "...applied as is..."

In an acute oral toxicity study conducted by Dow Chemical (1977), male rats (strain, age not provided) were treated once p.o. at doses of 126-2000 mg/kg (0.505-8.02 mmol/kg). Lethargy, convulsions, and tremors were observed among rats in the two high dose groups (1000 and 2000 mg/kg; 4.011 and 8.022 mmol/kg).

Results of an acute dermal irritation study in rabbits (strain, age not provided) indicate that a prolonged contact over 3 days is essentially non-irritating (Dow Chemical, 1977). Only one animal was used per treatment regimen. Results of an eye irritancy test in rabbits (strain, age not provided) indicate that this material may produce slight, transient conjunctival irritation (Dow Chemical, 1977).

9.1.4 Short-term and Subchronic Exposure

The details of this study are presented in **Table 3**.

Results of a dermal irritation study in rabbits (strain, age not provided) indicate that repeated contact (10 applications over 14 days) may produce slight irritation (Dow Chemical, 1977).

9.1.5 Chronic Exposure

No data on the effect of chronic exposure for triallyl isocyanurate were available.

9.2 Reproduction and Teratology

No data on the reproductive or teratological effects of triallyl isocyanurate were available.

9.3 Carcinogenicity

No carcinogenicity data were available for triallyl isocyanurate.

9.4 Genotoxicity

Studies for this section are presented in **Table 4**.

Table 3. Short-Term Exposure to Triallyl Isocyanurate

Species, Strain, and Age	Number and Sex of Animals	Chemical Form, Purity	Dose	Exposure/Observation Period	Results/Comments	Reference
Rabbit (strain, age n.p.)	3 rabbits; 1 rabbit/method Controls: None (sex n.p.)	Triallyl isocyanurate, purity n.p.	n.p. applied to (A) intact skin and (B) occluded skin	Method A: 10 applications over 14 d (intact skin). Method B: 10 applications over 14 d (occluded skin).	Repeated prolonged exposures may cause slight irritation.	Dow Chemical (1977)

Abbreviation: n.p. = not provided

Table 4. Genotoxicity of Triallyl Isocyanurate

Test System	Biological Endpoint	S9 Metabolic Activation	Chemical Form, Purity	Dose	Endpoint Response	Results/Comments	Reference
9.4.1. Prokaryote Systems							
<i>Salmonella typhimurium</i> strains TA97, TA98, TA100, TA1535, and TA 1537	<i>his</i> gene mutations	+/-	triallyl isocyanurate; 99+% pure	33-6666 µg/plate (0.13-26.74 µmol/plate)	+S9: negative	S9 prepared from livers from Aroclor 1254-induced male Sprague-Dawley rats and male Syrian hamsters.	Zeiger et al. (1992)
9.4.2. In Vitro Mammalian Genotoxicity Assays							
9.4.2.1 DNA Damage							
Chinese hamster ovary (CHO) cells	Sister chromatid exchanges (SCE)	+/-	triallyl isocyanurate; purity n.p.	-S9: 29.7-605.0 µg/mL (0.119-2.43 mM) +S9: 29.1-291.0 µg/mL (1.17-11.7 mM)	-S9: 24/24 ¹ = negative +S9: 2/24 ¹ = negative	Maximum dose based on toxicity.	Loveday et al. (1990)
9.4.2.2 Chromosomal Damage							
CHO cells	chromosomal aberrations	+/-	triallyl isocyanurate; purity n.p.	-S9: 0.146-1.46 mg/mL (0.586-5.86 mM) +S9: 0.291-2.91 mg/mL (1.17-11.7 mM)	-S9: 8/8 ¹ = negative +S9: 2/8 ¹ = negative	Maximum dose based on toxicity.	Loveday et al. (1990)
Chinese hamster lung (CHL) cells	chromosomal aberrations	+/-	triallyl isocyanurate; purity n.p.	+S9: 0.250-1.00 mg/mL (1.00-4.01 mM)	-S9: 24/24 ¹ = equivocal 48/48 ¹ = equivocal 6/24 ¹ = negative +S9: 6/24 ¹ = positive	Maximum dose based on obtaining ≥ 50% depression in cell growth.	Sofuni et al. (1990)

Abbreviations: n.p. = not provided; +/- = presence/absence
¹Time provided is for exposure duration followed by sample time after start of treatment.

Table 4. Genotoxicity of Triallyl Isocyanurate (continued)

Test System	Biological Endpoint	S9 Metabolic Activation	Chemical Form, Purity	Dose	Endpoint Response	Results/Comments	Reference
CHO cells	chromosomal aberrations	+/-	triallyl isocyanurate; purity n.p.	-S9: 0.146-1.46 mg/mL (0.586-5.86 mM) +S9: 0.291-2.91 mg/mL (1.17-11.7 mM) +S9: 200-500 µg/mL (0.802-2.01 mM)	-S9: 8/10.5 ¹ = negative +S9: 2/12 ¹ = negative +S9: 6/24 ¹ = positive	Doses matched those used by Loveday et al. (1990). Maximum dose based on obtaining > 50% depression in cell growth.	Sofuni et al. (1990)

Abbreviations: n.p. = not provided; +/- = presence/absence
¹Time provided is for exposure duration followed by sample time after start of treatment.

9.4.1 Prokaryote Systems

When tested for mutagenicity in *Salmonella typhimurium* strains TA97, TA98, TA100, TA1535, and TA1537, in the presence and absence of metabolic activation, triallyl isocyanurate was negative at doses ranging from 33 to 6666 µg/plate (0.13 to 26.74 µmol/plate) (Zeiger et al., 1992). Metabolic activation consisted of S9 prepared from livers collected from Aroclor 1254-induced male Sprague-Dawley rat and male Syrian hamsters.

9.4.2 In Vitro Mammalian Systems

9.4.2.1 DNA Damage

Triallyl isocyanurate, at doses up to 605 µg/mL (2.43 mM) and 291 µg/mL (1.17 mM) in the absence and presence of metabolic activation, respectively, did not induce sister chromatid exchanges (SCE) in Chinese hamster ovary (CHO) cells (Loveday et al., 1990).

9.4.2.2 Chromosomal Damage

Triallyl isocyanurate, at doses up to 1.46 mg/mL (5.86 mM) and 2.91 mg/mL (11.7 mM) in the absence and presence of metabolic activation, respectively, did not induce chromosomal aberrations in CHO cells when cells were sampled 8 to 10.5 hours after the start of treatment (Loveday et al., 1990; Sofuni et al., 1990). However, in CHO or Chinese hamster lung (CHL) cells, when sampling occurred 24 hours after the start of treatment, triallyl isocyanurate at doses up to 2.91 mg/mL (11.7 mM) and 1 mg/mL (4.01 mM), respectively, produced a clastogenic, dose-dependent response in the presence of metabolic activation (Sofuni et al., 1990).

9.4.3 In Vivo Mammalian Studies

No information pertaining to the genotoxicity of triallyl isocyanurate in *in vivo* mammalian systems was available.

9.5 Immunotoxicity

No data pertaining to the immunotoxicity of triallyl isocyanurate were available.

10.0 STRUCTURE-ACTIVITY RELATIONSHIPS

No information pertaining to the structure-activity relationships of triallyl isocyanurate was available.

11.0 ONLINE DATABASES AND SECONDARY REFERENCES**11.1 Online Databases**Chemical Information System Files

SANSS (Structure and Nomenclature Search System)

TSCATS (Toxic Substances Control Act Test Submissions)

DIALOG Databases

Chemical Economics Handbook

National Library of Medicine Databases

EMIC and EMICBACK (Environmental Mutagen Information Center)

STN International Datafiles

AGRICOLA

BIOSIS

CANCERLIT

CAPLUS

CHEMLIST

EMBASE

HSDB

LIFESCI

MEDLINE

PROMPT

Registry

RTECS

TOXLINE

TOXLINE includes the following subfiles:

Toxicity Bibliography	TOXBIB
International Labor Office	CIS
Hazardous Materials Technical Center	HMTC
Environmental Mutagen Information Center File	EMIC
Environmental Teratology Information Center File (continued after 1989 by DART)	ETIC
Toxicology Document and Data Depository	NTIS
Toxicological Research Projects	CRISP
NIOSHTIC7	NIOSH
Pesticides Abstracts	PESTAB

Poisonous Plants Bibliography	PPBIB
Aneuploidy	ANEUPL
Epidemiology Information System	EPIDEM
Toxic Substances Control Act Test Submissions	TSCATS
Toxicological Aspects of Environmental Health	BIOSIS
International Pharmaceutical Abstracts	IPA
Federal Research in Progress	FEDRIP
Developmental and Reproductive Toxicology	DART

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ACKNOWLEDGMENTS

Support to the National Toxicology Program for the preparation of the Toxicology of Triallyl Isocyanurate—Review of Literature was provided by Integrated Laboratory Systems, Inc., through NIEHS Contract Number N01-ES-65402. Contributors included: Raymond R. Tice, Ph.D. (Principal Investigator); Brigette D. Brevard, M.A. (Co-Principal Investigator); Maria S. Donner, Ph.D.; Esther M. Morris, M.S.; Claudine A. Gregorio, M.A.; and Bonnie L. Carson, M.S.