ALLYL BROMIDE
CAS NO. 106-95-6

Structure, Molecular Formula and Molecular Weight:

$BrCH_2CH=CH_2$

C_3H_5Br Mol. wt.: 120.98

BASIS OF NOMINATION TO THE CSWG
The nomination of allyl bromide (AB) to the CSWG is based on potential for human exposure and suspicion of carcinogenicity.

AB is an industrial and research chemical with evidence of widespread use. Although annual production volumes could not be established from the available literature, a large number of companies are reported as producers or suppliers of unspecified amounts of AB. AB is also a documented environmental pollutant. AB is an alkylating agent, which is reported to be mutagenic in the Ames/Salmonella assay and is shown to bind to DNA. As an allyl halide, AB is structurally related to allyl chloride, which was reported to be negative in male and female rats, and equivocal in male and female mice in NCI/NTP carcinogenicity studies. However, allyl bromide would be expected to be a better alkylating agent than allyl chloride.

SELECTION STATUS
ACTION BY CSWG: 12/16/94
Studies Requested: Carcinogenicity
Priority: Moderate
Rationale/Remarks:

- Potential for human exposure
- Widespread use
- Environmental pollutant
- Suspicion of carcinogenicity
- Alkylating agent
- Positive genotoxicity test results
- Test by inhalation, the most likely route of human exposure

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INPUT FROM GOVERNMENT AGENCIES/INDUSTRY

Dr. John Walker, Director, TSCA Interagency Testing Committee (ITC), reported to TRI that AB has been deferred based on a lack of reported annual production volumes of greater than 10,000 pounds per individual producer in 1989.

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SUMMARY OF DATA FOR CHEMICAL SELECTION

CHEMICAL IDENTIFICATION

CAS Registry No.:	106-95-6
Chemical Abstract Name:	1-Propene, 3-bromo-
Synonyms:	Allyl bromide; propene, 3-bromo-; 3-bromopropene; 3-bromopropylene; 2-propenyl bromide; AB

Chemical and Physical Properties:

Description:	Colorless to faintly yellow clear liquid with an unpleasant, pungent odor (Budavari, 1989; Lewis, 1993; Anon., 1994a).
Boiling Point:	70°C at 752 mm (Lide, 1993)
Melting Point:	-119°C (Lide, 1993)
Density:	1.398 at 20°C / 4°C (Lide, 1993)
Refractive Index:	1.4654 (Lewis, 1993)
Vapor Density (air=1):	4.2 (Anon., 1984)
Flash Point:	-1.1°C (Lewis, 1993)
Solubility:	Slightly soluble in water; soluble / miscible with carbon disulfide, carbon tetrachloride, chloroform, diethyl ether, and ethanol (Budavari, 1989; Lide, 1993; Lewis, 1993).
Stability:	Normally stable but can become unstable at elevated temperatures (Anon., 1993)
Log P (octanol / water partition coefficient):	1.74 (Nielsen & Bakbo, 1985); 1.59 (Lipnick et al., 1987)
Hydrolysis rate (tΩ):	2.5 hours in H_2O at 37°C (Nielsen & Bakbo, 1985)
Reactivity:	May react with water with some release of energy but not violently (Anon., 1993). Dangerous fire and explosion hazard when exposed to heat, flame or oxidizers. When heated to decomposition it emits toxic bromide fumes (Sax & Lewis, 1989).

Technical Products and Impurities: Allyl bromide (AB) is commercially available with a purity of 99% from Morre-Tec Industries, Inc. (Anon., 1994b). Aldrich Chemical Co. offers AB with a purity of 99% (98.5% min.) or 97% (96.5% min.) (Anon., 1994a). Chemstaff, Inc. also offers 99.0% pure AB with up to 0.5% low boiling impurities and up to 0.5% high boiling impurities (including allyl alcohol).

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EXPOSURE INFORMATION

Commercial Availability

Production and Producers: Allyl bromide is prepared by treating allyl alcohol with a bromide and sulfuric acid. It can also be made by the partial dehydrobromination of dibromopropane in a high-temperature cracking reaction (Stenger, 1978; Matheson, 1991).

AB is listed on the US EPA's TSCA Inventory (STN, 1994). AB is a significant industrial and research chemical for which bulk price listings are included regularly in the Chemical Prices section of the chemical industry weekly newspaper, Chemical Marketing Reporter. However, no annual production volumes were found in the available literature, including Synthetic Organic Chemicals, US Production and Sales which does not track AB as an individual chemical. According to Dr. John Walker of the Interagency Testing Committee (ITC), AB was placed on deferred status because of a lack of reported annual production volumes of greater than 10,000 lbs. per individual producer in 1989 (Walker, 1994).

In the most current chemical industry directories for 1993-94, the following eight companies are listed as producers of AB: Aldrich Chemical Co.; Chemstaff, Inc.; Dajac Laboratories; Morre-Tec Industries, Inc.; Narchem Corp.; Rhone-Poulenc, Inc.; SAF Bulk Chemicals; Spectrum Chemical Mfg. Co./Janssen Chimica.

Additional companies listed in recent directories of the last five years, DIALOG's Fine Chemicals Database (FCDB), or the Hazardous Substances Data Bank (HSDB) include the following: Ameribrom, Inc.; American Hoechst Corp.; American Tokyo Kasei; J.T. Baker, Inc.; Chemical Dynamics Corp.; Chem Service, Inc.; Columbia Organic Chemicals Co.; Crescent Chemical Co., Inc.; D & O Chemicals, Inc.; Eastman Kodak Co.; EM Science; Ethyl Corp./Hardwicke Chemical Co.; Fairfield Chemical Co.; Freeman Industries, Inc.; Jonas Chemical Corp.; E.B. Knight, Inc.; Lancaster Synthesis, Ltd.; Mallinckrodt, Inc.; Pfaltz & Bauer, Inc.; Sigma Chemical Co.; White Chemical Corp.

According to the TSCA Plant and Production database (TSCAPP, 1983), annual production/importation data reported for 1977 included the following: Columbia Organic Chemicals Co. produced 1,000 to 10,000 lbs and imported 1,000 to 10,000 lbs of AB; Freeman Industries, Inc., imported 1,000 to 10,000 lbs; American Hoechst Corp. declared importation of an unspecified volume.

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The following additional companies are listed as worldwide manufacturers or suppliers of AB:

Anachemia Canada Inc.
Asia Associates, Inc.
BDH Chemicals Ltd.
Dixon Fine Chemicals
Fluka Chemie AG
Fuji Pure Chemicals Co.
Ichikawa Gosei Chemical Co. Ltd.
Kock-Light Ltd.
Laborat Gesellschaft fur Laborchemikalien mbH
Manac Inc.
Monomer-Polymer and Dajac Labs., Inc.
Nacalai Tesque, Inc.
National Chemical Corporation
Potasse & Produits Chimiques S.A.
Riedel-de Haen AG
Teijin Chemicals Ltd.
Dr. Theodor Schuchardt & Co.
Tosoh Corporation

Imports: Besides the TSCAPP data on imports cited above, reports of importation of AB from several Western European countries totalled about 5,000 lbs in 1993, according to the Journal of Commerce Piers Imports database (Dialog, 1994).

Use Pattern: AB is considered an industrially important organic bromine compound which is used extensively in organic and biochemical syntheses. McMahon et al. (1979) of Lilly Research Laboratories described AB as a common reagent and synthetic intermediate. Principal use categories for AB include: starting material/chemical intermediate in organic synthesis and intermediate in the manufacture of polymers/resins, synthetic perfumes, pharmaceuticals, agricultural chemicals (Kim et al., 1992; Kirimo et al., 1980), and other allyl compounds (Budavari, 1989; Stenger, 1978). It has been described as an insecticidal fumigant used in crop protection (Gosselin, 1984; Stenger, 1978). However, a representative of the National Agricultural Chemicals Association, in response to an inquiry, checked a list of chemicals with current fumigant use and did not find AB listed (Cannon, 1994).

Human Exposure: Potential for human exposure arises from its use in the manufacture of synthetic perfumes and other industrial/commercial synthetic products, including polymers and resins. Possible routes of entry include inhalation, ingestation or skin contact (Sittig, 1985). Sanduja et al. (1989) have suggested the use of urinary hydroxypropyl-mercapturic acid as a biological marker useful in monitoring of workers for exposure to several allylic compounds, including AB.

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Environmental Occurrence: AB is not known to occur naturally. However, AB has been identified as a pyrolytic degradation product of the brominated polymers, poly(dibromopropyl acrylate) and poly (dibromo-propylmethacrylate) (Grassie et al., 1986).

AB has also been documented as a pollutant of both air and water.

- AB was one of a group of organohalogen compounds identified in seven sources of wastewater or drinking water by researchers at UCLA (Bauman & Stenstrom, 1989).
- AB was identified as a major photolytic degradation product of aqueous 1,2-dibromopropane in both the absence and presence of hydrogen peroxide. In the absence of water, the yield of AB was 25% relative to the initial 1,2-dibromopropane present as a water contaminant in trace amounts (Milano & Vernet, 1988).
- According to Dunn et al. (1987), researchers at the University of Illinois, AB was one of 78 toxic volatile organic compounds routinely monitored in ambient air by mass spectral analysis.
- In a Russian study, AB was reported to be one of a group of ecologically significant air contaminants determined by gas chromatography (GC) (Zenkevich & Konyukhova, 1992).
- AB is listed in EPA's volatile organic chemicals (VOC) database (Database number: 107) (Shah & Singh, 1988).

Regulatory Status: The State of Pennsylvania lists AB as a hazardous substance tracked as a potential workplace hazard (Shafer, 1995). AB is regulated by the Department of Transportation (DOT) as a flammable liquid (DOT #1099) (Shafer, 1995; STN 1994).

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EVIDENCE FOR POSSIBLE CARCINOGENIC ACTIVITY

Human Data: No epidemiological studies or case reports investigating the association of exposures to AB and cancer risk in humans were identified in the available literature. AB is an irritant to skin, eyes and mucous membranes and is absorbed through the skin. Long term exposure has been found to cause hepatic and renal damage (Anon., 1989).

Volk et al. (1992) of the Bristol-Myers Squibb Company's Pharmaceutical Research Institute reported working to develop a rapid screening test to identify potential human carcinogens using pyridine ion as indicator. They found a good correlation between gas-phase reactivity of a variety of electrophiles with possible carcinogenic potency. AB was one of this group of chemicals which they considered potentially carcinogenic to humans.

Animal Data: No 2-year carcinogenicity studies of AB in animals were identified in the published literature. The Registry of Toxic Effects of Chemical Substances (RTECS) has reported toxicity data for AB as follows (NLM, 1994):

rat oral LD50 = 120 mg/kg
mouse ip LD50 = 48 mg/kg
rat inhalation LC50 = 10 gm/m3/30 mm
mammal inhalation LC50 = 4.11 gm/m3

AB is highly toxic to animals and fish. Concentrations as low as 1 mg/l reportedly caused fatal lung injury to experimental animals exposed for 4 hours (Gosselin, 1984). Nielsen and Bakbo (1985) reported that AB was a pulmonary irritant in mice exposed for 20-30 minutes. They determined a plateau value for the concentration inducing a 50% decrease in the respiratory frequency (RD50) to be 257 ppm in CF-1 mice exposed for 30 minutes.

AB has also been reported highly toxic to aquatic species (Lipnick et al., 1987). Of a group of 33 industrial water pollutants tested for acute toxicity to the clawed toad (Xenopus laevis), AB was one of the most highly toxic, with a 48 hour LC50 of 0.66 mg/l (de Zwart & Slooff, 1987). In another study of the acute aquatic toxicity of a large group of petroleum derived chemical pollutants, Bridie et al. (1979) reported that AB has an LC50 of < 0.8 mg/l, and is one of the most toxic to goldfish.

Short-Term Tests: AB was reported mutagenic in a modified Ames/Salmonella assay using strain TA100 (Eder et al., 1980). According to Eder et al. (1987b), AB is a direct acting mutagen which gave a test result of 700 rev/µmol without the addition of S9. Lijinsky and Andrews

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(1980) also reported AB to be mutagenic in S. typhimurium strain TA100 in the absence of metabolic activation; the addition of S9 largely eliminated the mutagenic activity.

Schiffmann et al. (1983) reported, in addition, that AB induced unscheduled DNA synthesis (UDS) in HeLa S3 cells with a dose dependent mode of action. Eder et al. (1983) found nearly linear quantitative correlations between mutagenicity and alkylating properties and between mutagenicity and genotoxic effects in the UDS.

As part of a battery of tests to explore direct as well as indirect genotoxicity of AB, Eder et al. (1982) studied in vitro DNA binding through alkylation of salmon sperm DNA. Their results indicated that AB binds to DNA yielding the five allyl substituted nucleic bases: N2-allylguanine, O6-allylguanine, N7-allylguanine, N3-allyladenine and N6-allyladenine. In an in vivo DNA binding study in which 14C labelled AB was administered by gavage to mice, all five allylated nucleic bases were identified in hydrolysate DNA from different organs indicating direct genotoxicity of AB in the whole animal (Eder et al., 1983; Eder et al., 1986). Eder et al. (1986) also reported an in vitro binding half-life of 54 for AB at 37°C of 8.1 hours and alkylating activity (-E560nm) based on a 4-(p-nitrobenzyl) pyridine (NBP) test.

Metabolism: Kaye et al. (1972) studied allyl halide metabolism in male rats. After the animals were treated subcutaneously with AB, 3-hydroxypropylmercapturic acid, allylmercapturic acid and its sulfoxide were reportedly excreted in the urine. According to the authors, these metabolites can be formed by a number of different pathways because allyl halides can undergo reactions at either the double bond or the halide bonding site. Eder et al. (1986) performed metabolism studies on allyl compounds, including AB, as part of a screening strategy to investigate genotoxic potential. They also reported that allylic compounds which are alkylating agents, are detoxified via substitution reactions with glutathione (GSH) to produce mercapturic acids. In addition, they reported that AB undergoes metabolic transformation to acrolein as a reactive intermediate; however, AB does not appear to be metabolized via an epoxide route. The metabolic pathways proposed for AB are shown schematically below.

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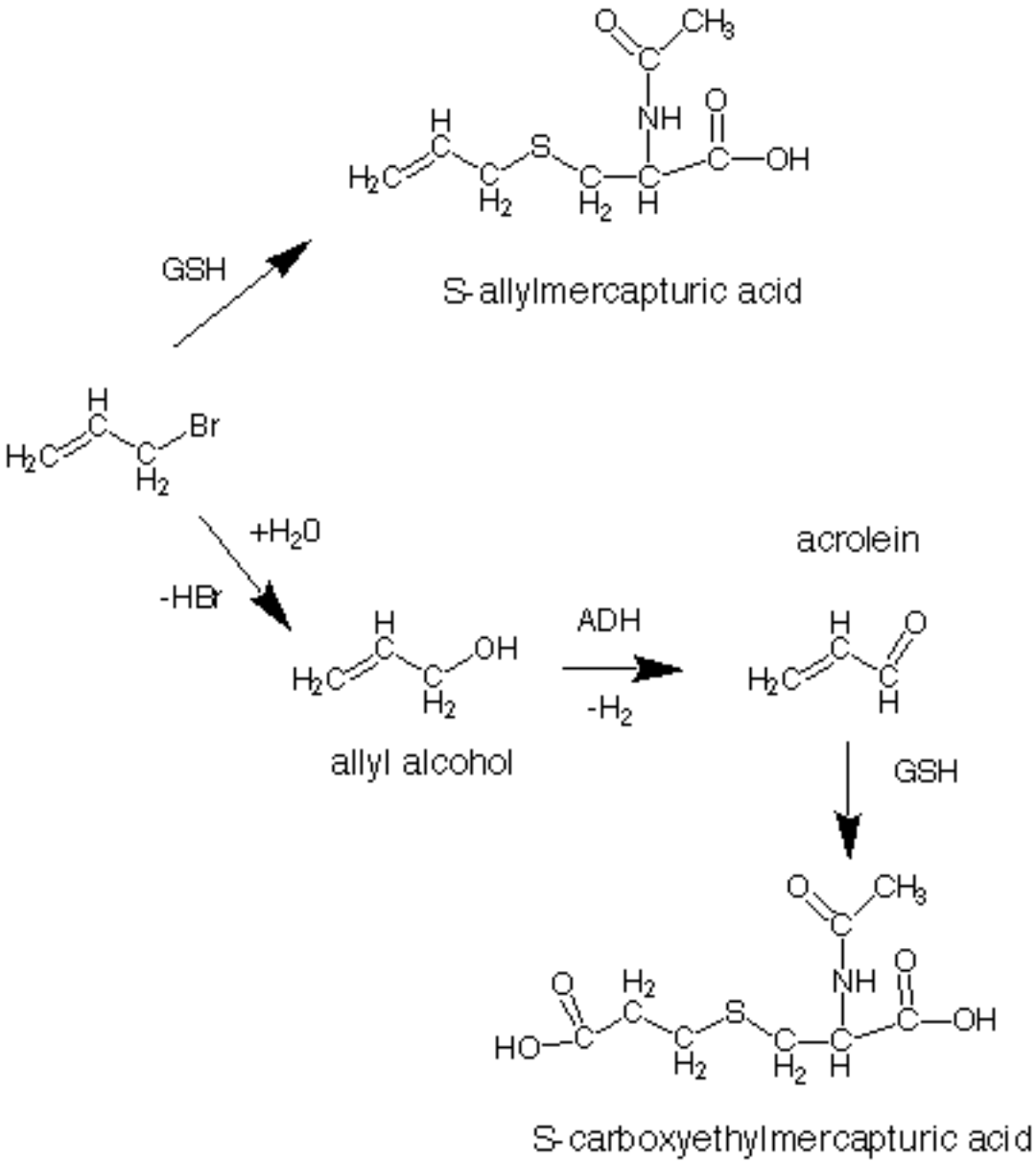
[A diagram "Metabolic pathways for allyl bromide (Eder et al., 1986) appeared in original document but was lost in translation from WordPerfect to Word - see paper copy of document in Central Files]



Other Biological Effects: AB has been shown to be a reactive electrophile and an alkylating agent. Patel et al. (1981) reported that AB was one of a group of allylic industrial toxicants capable of destroying hepatic cytochrome P-450.

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Structure/Activity Relationships: Unsaturated aliphatic halides are among the halogenated organics which have been extensively studied because of their mutagenic and DNA-modifying effects. A group of analogs structurally similar to AB were screened for data relevant to the possible association, either positively or negatively, of mutagenicity or carcinogenicity with compounds of this structural type. Structures for the analogs considered are shown in Appendix A. Two AB analogs, allyl chloride and 3-chloro-2-methylpropene, have been tested by the NTP with the following results (NTP, 1994):

- Allyl chloride [107-05-1] [a] was mutagenic in an Ames/Salmonella assay. In NTP carcinogenicity studies, this chemical was found negative in male and female rats and equivocal in male and female mice. IARC evaluated this chemical and placed it in Group 3 (agent is not classifiable as to its carcinogenicity to humans) based on no data for evaluation in humans and inadequate data for evaluation in experimental animals (IARC, 1985a).

- 3-Chloro-2-methylpropene (methyl allyl chloride) [563-47-3] [c] was tested in a battery of short-term genetic toxicity tests with a range of results reported as follows: weakly positive for mutagenicity in S. typhimurium strain, TA1537 with rat liver S9, equivocal in TA100 with both rat and hamster liver S9, and negative in TA1535 and TA98 both with and without metabolic activation; positive in a mouse lymphoma (ML) L5178Y/TK+/- forward mutation assay without activation; positive for induction of chromosomal aberrations (CAs) and sister chromatid exchanges (SCEs) without activation in Chinese hamster ovary (CHO) cells; negative in a micronucleus (MN) test; positive for sex-linked recessive lethal (SLRL) mutations but negative for reciprocal translocations in Drosophila melanogaster. In NTP carcinogenicity studies, this chemical was reported to produce clear evidence of carcinogenicity (increased forestomach squamous cell neoplasia) in male and female rats and male and female mice (NTP, 1986; Foureman et al., 1994).

1,3-Dichloropropene [542-75-6] [d] was evaluated by IARC and classified in Group 2B (the agent (mixture) is possibly carcinogenic to humans) based on inadequate data (I) for evaluation in humans but sufficient data (S) for evaluation in experimental animals (IARC, 1986; IARC, 1987). The exposure circumstances entail exposures that are possibly carcinogenic to humans. Another analog, 1,4-dichloro-2-butene [764-41-0] [e], is reported to be a nasal tumorigen in rats, according to Bos et al. (1992). However, IARC evaluated this chemical and placed it in Group 3 (agent cannot be classified as to its carcinogenicity to humans) based on no data (ND) for evaluation in humans and inadequate data (I) for evaluation in experimental animals (IARC, 1977; IARC, 1987).

Schiffmann et al. (1983) studied the induction of unscheduled DNA synthesis (UDS) in HeLa cells by the incorporation of [^{3}H]thymidine. UDS occurred at lower concentrations of allyl iodide (171 x 10^6 cells at 50 µM) than for AB (406 x 10^6 cells at 500 µM) or allyl

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chloride (152 x 10^6 cells at 1000 µM). UDS activity correlated with mutagenicity in Salmonella typhimurium for these three simple allyl halides. However, the mutagenicity of AB exceeded that of other allyl compounds with equal or greater UDS activity. Allylic compounds with greater UDS activity but lower mutagenicity than AB include cis- and trans-1,3-dichloropropene [10061-01-5; 10061-02-6] [d], 1-chloro-2-butene [4894-61-5] [g], and 2,3-dichloro-1-propene [78-88-6] [h].

The direct binding of AB and allyl chloride to DNA was demonstrated by Eder et al. (1987b). The half-life of the alkylation reaction was much shorter for AB (8.1 vs. 360 hours) but the same alkylated products were detected by HPLC, including N^3-allyladenine, N^6-allyladenine, N^2-allylguanine, N^7-allylguanine, and O^6-allylguanine; several other unidentified compounds were also formed.

Using isolated rat liver perfused with solutions containing either AB or allyl chloride, Eder and Zugelder (1990) demonstrated the in vivo formation of the five adducts described above. The authors suggested that the formation of allyl adducts, especially the promutagenic O^6-guanine adduct, clearly indicates that the cancer-initiating potential of these compounds must be considered.

Eder et al. (1987a) determined that neither AB nor allyl chloride was metabolized via an epoxide pathway in rats. The metabolism of both compounds was similar and included the production of S-carboxyl mercapturic acid, the principal metabolite of the mutagen, acrolein. It is likely that direct alkylation of GSH also occurs in vivo, resulting in the direct formation of the non-mutagenic mercapturic acids. While the mutagenicity of AB and allyl chloride is decreased by incubation with S9, the mutagenicity of 2,3-dichloro-1-propene is enhanced. The strongly mutagenic 1,3-dichloroacetone, formed by rearrangement of the unstable epoxide intermediate, represents 3-4% of the total urinary metabolites in rats; the even stronger mutagen, 2-chloroacrolein, was also detected as a metabolite of 2,3-dichloro-1-propene.

Lipnick et al. (1987) examined the relative acute toxicity of several allylic compounds to goldfish. LC_{50}s were obtained for 3-chloro-2-methyl propene (14 mg/l), allyl chloride (10 mg/l), AB (0.8 mg/ml), and allyl alcohol (1 mg/ml). The toxicity of all four allylic compounds was greater than that predicted based on the respective octanol/water partition coefficients (log P: 3-chloro-2-methyl propene [563-47-3] [c], 1.849; AB, 1.590;

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allyl chloride [a];1.450). The authors interpreted the excess toxicity of AB, allyl chloride, and 3-chloro-2-methyl propene to be related to the S_N2 nucleophilic substitution reaction mechanism common to these compounds. Reaction rates for nucleophilic substitutions at the activated allylic carbon proceeding by the S_N2 mechanism are related to the stability of the leaving group as a free moiety. Because bromide is a better leaving group than chloride, the toxicity of AB is greater than that of allyl chloride, even though the two compounds have similar partition coefficients.

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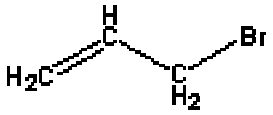
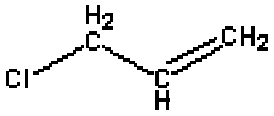
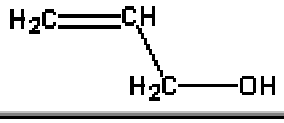
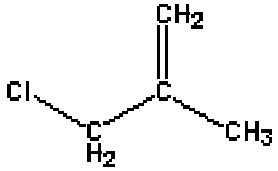
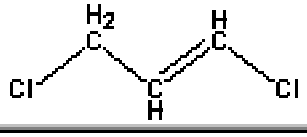
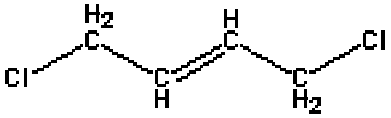
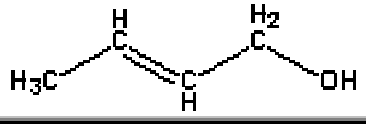
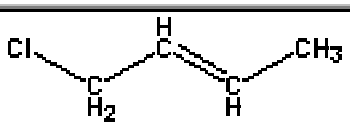
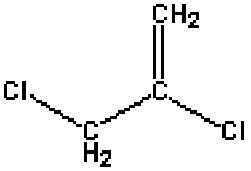
["Appendix A: Allyl Bromide and structurally related compounds" appeared here in the original document but was lost in reformatting from WordPerfect to Word - see original document on file in the Central Files.]

Appendix A. Allyl bromide and structurally related compounds

Allyl Bromide
106-95-6



Allyl Chloride	107-05-1	
Allyl Alcohol	107-18-6	
3-Chloro-2-methylpropene	563-47-3	
1,3-Dichloropropene	542-75-6	
1,4-Dichloro-2-butene	764-41-0	
Crotyl Alcohol	6117-91-5	
1-Chloro-2-butene	591-97-9	
2,3-Dichloro-1-propene	78-88-6	

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REFERENCES

Anon. (1984) Fire Protection Guide on Hazardous Materials, 8th ed., National Fire Protection Association, Quincy, MA

Anon. (1989) Chemical Safety Monograph, National Board of Labour Protection (Finland), International Occupational Safety and Health Information Centre, Geneva, Switzerland

Anon. (1994a) Chemical Specification Sheet: Allyl Bromide (Product Number: a 2958-5 & 33752-8), Aldrich Chemical Co., Milwaukee, Wisconsin

Anon. (1994b) Product Specification Sheet: Allyl bromide, Morre-Tec Industries, Inc., Carteret, New Jersey

Ashby, J. & Paton, D. (1993) The influence of chemical structure on the extent and sites of carcinogenesis for 522 rodent carcinogens and 55 different human carcinogen exposures, Mutat. Res., 286(1):3-74

Bauman, L. & Stenstrom, M.K. (1989) Observations of the reaction between organohalides and sulfite, Environ. Sci. Technol., 23(2):232-6

Bos, P.M.J., Zwart, A., Reuzel, P.G.J. & Bragt, P.C. (1992) Evaluation of the sensory irritation test for the assessment of occupational health risk, Crit. Rev. Toxicol., 21(6):423-450

Bridie, A.L., Wolff, C.J.M. & Winter, M. (1979) The acute toxicity of some petrochemicals to goldfish, Water Res., 13(7):623-626

Budavari, S., ed. (1989) The Merck Index, 11th ed., Merck & Co., Inc., Rahway, NJ

Cannon, D.J. (1994) Telephoned report from Raymond McAlister, National Agricultural Chemicals Association (NACA) Washington, DC, to Dorothy Cannon of Technical Resources International, Inc. (TRI), 3/23/94

CIS (1994) TSCA, Plant and production (TSCAPP) database, Chemical Information Systems, a division of PSI International, Inc., Towson, MD.

de Zwart, D. & Slooff, W., (1987) Toxicity of mixtures of heavy metals and petrochemicals to Xenopus laevis, Bull. Environ. Contam. Toxicol., 38:345-351

Dialog (1994) PIERS Imports (U.S. Ports), database file 573, Dialog Information Services, Inc., Palo Alto, CA

Dunn, W.J. III, Koehler, M.G., Emery, S.L. & Scott, D.R. (1987) Application of pattern recognition to mass spectral data of toxic organic compounds in ambient air, Chemom. Intell. Lab. Syst., 1(4):321-34

Eder, E. & Zugelder, J.-P. (1990) DNA-binding studies with allylchloride and allylbromide using the isolated perfused rat liver technique, Toxicol. in Vitro, 4(4-5):661-665

Eder, E., Dornbusch, K. & Fischer, G (1987a) The role of biotransformation in the genotoxicity of allylic compounds, Arch. Toxicol., 60:182-6

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)

Eder, E., Henschler, D. & Neudecker, T. (1982) Mutagenic properties of allylic and , -unsaturated compounds: consideration of alkylating mechanisms, Xenobiotica, 12(12):831-848
Eder, E., Lutz, D. & Henschler, D. (1981) In vitro alkylation of DNA by mutagenic allyl compounds, Arch. Pharmacol., 316(Suppl.):R13

Eder, E., Lutz, D. & Jˆrns, M. (1987b) Allylic compounds bind directly to DNA: investigation of the binding mechanisms in vitro, Chem. Biol. Interact., 61(2):97-108

Eder, E., Neudecker, T., Lutz, D. & Henschler, D. (1980) Mutagenic potential of allyl and allylic compounds. Structure-activity relationship as determined by alkylating and direct in vitro mutagenic properties, Biochem. Pharmacol., 29(7):993-998

Eder, E. Schiffmann, D., Dornbusch, K., K¸tt, W. & Hoffman, C. (1986) Genotoxicity of allyl compoundsóa quick screening strategy based on structure-activity relationships and a battery of prescreening tests, Food Chem. Toxicol., 24(6-7):667-673

Eder, E., Schiffmann, D., Neudecker, T. & Henschler, D. (1983) Dependence of direct genotoxic activities of allylic compounds on their alkylating properties, J. Cancer Res. Clin. Oncol., 105(2):A17

Foureman, P., Mason, J.M., Valencia, R. & Zimmering, S. (1994) Chemical mutagenesis testing in Drosophila. X. Results of 70 coded chemicals tested for the National Toxicology Program, Environ. Molec. Mutagen., 23(3):208-227

Gosselin, R.E., Smith, R.P. & Hodge, H.C. (1984) Clinical Toxicology of Commercial Products, 5th ed., Williams & Wilkins, Baltimore, MD

Grassie, N., Diab, M.A.M. & Scotney, A. (1986) Thermal degradation of bromine-containing polymers. Part 7. Poly (2,3-dibromopropyl methacrylate) and poly (2,3-dibromopropyl acrylate), Polym. Degrad. Stab., 16(1):79-97 [STN abstract, CA 106:33571x]

IARC (1977) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Vol. 15, Miscellaneous industrial chemicals, Lyon, pp.149-153

IARC (1985a) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Vol. 36, Allyl Compounds, Aldehydes, Epoxides and Peroxides, Lyon, pp.31-34, 39-54

IARC (1985b) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Vol. 39, Some Chemicals Used in Plastics and Elastomers, Lyon, pp.133-145

IARC (1986) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Vol. 41, Some Halogenated Hydrocarbons, Lyon, pp.113-128

IARC (1987) IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans, Suppl 7, Overall Evaluation of Carcinogenicity: An Updating of IARC Monographs Volumes 1 to 42, Lyon, pp. 62-73

Kaye, C.M., Clapp, J.J. & Young, L. (1972) The metabolic formation of mercapturic acids from allyl halides, Xenobiotica, 2(2):129-139

Kim, J.N., Kim, K.M. & Ryu, E.K. (1992) Improved synthesis of N-alkoxyphthalimides, Synth. Commun., 22(10):1427-1432

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)

Kirino, O., Oshita, H., Oishi, T. & Kato, T. (1980) Preventive activities of N-substituted- -aminonitriles against Fusarium diseases, Agric. Biol. Chem., 44(1):25-30

Lewis, R.J., Sr., ed. (1993) Hawley's Condensed Chemical Dictionary, 12th ed., New York, Van Nostrand Reinhold Co., p. 39

Lide, D.R., ed. (1993) CRC Handbook of Chemistry and Physics, 74th ed., Boca Raton, FL, CRC Press, Inc., pp. 3-31

Lijinsky, W & Andrews, A.W. (1980) Mutagenicity of vinyl compounds in Salmonella typhimurium, Teratogen. Carcinogen. Mutagen., 1:259-267

Lipnick, R.L., Watson, K.R. & Strausz, A.K. (1987) A QSAR study of the acute toxicity of some industrial organic chemicals to goldfish. Narcosis, electrophile and proelectrophile mechanisms, Xenobiotica, 17(8):1011-25

Matheson, D. (1991) Allyl compounds. In: Encyclopaedia of Occupational Health and Safety, Vol. 1, 3rd ed., International Labour Organization, Geneva, pp. 128-129

McMahon, R.E., Cline, J.C. & Thompson, C.Z. (1979) Assay of 855 test chemicals in ten tester strains using a new modification of the Ames test for bacterial mutagens, Cancer Res., 39:682-693

Milano, J.C. & Vernet, J.L. (1988) Photolytic degradation of 1,2-dibromopropane present in trace amounts in water - effect of hydrogen peroxide, Chemosphere, 17(5):963-71

Nielsen, G.D. & Bakbo, J.C. (1985) Sensory irritating effects of allyl halides and a role for hydrogen bonding as a likely feature at the receptor site, Acta Pharmacol. Toxicol., 57:106-116

NLM (1994) National Library of Medicine, Toxicology Data Network (TOXNET) information Services, databases searched (see search resource list)

NTP (1986) Toxicology and carcinogenesis studies of 3-chloro-2-methylpropene in F344 rats and B6C3F1 mice (gavage studies). National Toxicology Program, Technical Report Series #300, U.S. Department of Health and Human Services, Bethesda, MD

NTP(1994) NTP Management Status Report, NTP Chemtrack system, National Toxicology Program, National Institute of Environmental Health Sciences, Research Triangle Park, NC

Patel, J.M. et al. (1981) Destruction of hepatic cytochrome P-450 by allylic industrial toxicants, FASEB 65th annual meeting, Fed. Proc. 40 (3 Part 1):636

Sanduja, R., Ansari, G.A.S. & Boor, P.J. (1989) 3-Hydroxypropylmercapturic acid: a biological marker of exposure to allylic and related compounds, J. Appl. Toxicol., 9(4):235-8

Sax, N.I. & Lewis, R.J. Sr. (1989) Dangerous Properties of Industrial Materials, 7th Ed., Vol. 2, New York, Van Nostrand Reinhold, p. 114

Schiffmann, D., Eder, E., Neudecker, T. & Henschler, D. (1983) Induction of unscheduled DNA synthesis in HeLa cells by allylic compounds, Cancer Lett., 20:263-9

Shafer, D. (1995) The Book of Chemical Lists, Vol. II, Business & Legal Reports, Inc., Madison, CT., p. 15-8

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)

Shah, J. & Singh, H.B. (1988) Distribution of volatile organic chemicals in outdoor and indoor air, Environ. Sci. Technol., 22(12):1381-1388

Sittig, M. (1985) Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2nd. ed, Noyes Publications, Park Ridge, NJ

Stenger, V.A. (1978) Bromine compounds. In: Grayson, M., ed. Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed., Vol. 4, pp. 256-9, John Wiley & Sons, New York

STN (1994) The Scientific & Technical Information Network, STN International, databases searched (see search resource list)

Volk, K.J., Yost, R.A., Brajter-Toth, A. & Freeman, J.A. (1992) A dynamic approach for studying redox reactions: electrochemistry on-line with mass spectrometry, Analysis, 20(7):421-5

Walker, J.D. (1994) Direct communication by telephone call between Dr. John Walker, Executive Secretary of the TSCA Interagency Testing Committee (ITC) and Dorothy Cannon of Technical Resources, Inc., February 15, 1994

Zenkevich, I. & Konyukhova, S.V. (1992) Gas chromatographic identification of ecologically safe freons, Vestn. St.-Peterb. Univ., Ser. 4: Fiz. Khim., (1):66-70 [STN Abstr. 118:174663]

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)

Summary Sheet Checklist for Allyl bromide (106-95-6)

NLM

CCRIS

EMIC

EMICBACK

GENETOX

HSDB

IRIS

RTECS

TOXLINE

TOXLINE65

TOXLIT

TRI89

TRI90

STN INTERNATIONAL

BIOSIS-RN

CA / CAOLD

CA PREVIEWS

CBNB

CIN

CHEMLIST

HODOC

NIST THERMO

REGISTRY

CIS

TSCAPP

DIALOG

NIOSH / OSHA (161)

Chapman & Hall Chemical Database (303)

Chemical Safety NewsBase (317)

Fine Chemicals Database (360)

Piers Imports (573,574)

MANUAL SOURCES

Amdur, M.O., Doull, J. & Klassen, D.C., eds. (1991) Casarett and Doull's Toxicology. The Basic Science of Poisons, 4th ed., Macmillan Publishing Co., New York

Budavari, S., ed. (1989) The Merck Index, 11th ed., Merck & Co., Inc., Rahway, NJ (available online as Merck Online, DIALOG file #304)

Chemical Company Guides and Directories

Aldrich Catalog / Handbook of Fine Chemicals
Chemcyclopedia
Chemical Week Buyers' Guide
Janssen Chimica Catalog
Mallinkrodt Chemicals Catalog (available online as MALLIN)
OPD Chemical Buyers Directory

Gilman, A.G., Goodman, L.S., Rall, T.W. & Murad, F., Eds. (1985) Goodman and Gilman's The Pharmacological Basis of Therapeutics, 7th ed., Macmillan Publishing Co., New York

Grayson, M., ed. (1978-1984) Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed., John Wiley & Sons, Inc., New York (available online as Kirk-Othmer Online, DIALOG file #302)

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)

IARC (1994) Directory of Agents Being Tested for Carcinogenicity, Number 16, International Agency for Research on Cancer, World Health Organization, Lyon, France

Lewis, R.J., Sr. (1993) Hawley's Condensed Chemical Dictionary, 12th ed., Van Nostrand Reinhold Co., New York

Lide, D.R. ed., (1993) CRC Handbook of Chemistry and Physics, 74th ed., CRC Press, Inc., Boca Raton, FL

National Cancer Institute (1994) Division of Cancer Etiology Short Term Test Program Results tracking file

National Toxicology Program (1994) NTP Results Report: Results and Status Information on All NTP Chemicals, April 8, 1994 Report

PHS-149 (1951-1992) Survey of Compounds Which Have Been Tested for Carcinogenic Activity, National Cancer Institute, U.S. Department of Health and Human Services, Bethesda, MD

Sax, N.I. & Lewis, R.J., Sr. (1987) Hazardous Chemicals Desk Reference, Van Nostrand Reinhold Co., New York

Sittig, M. (1981) Handbook of Toxic and Hazardous Chemicals, Noyes Data Corporation, Park Ridge, NJ

Original prepared for NCI by Technical Resources International, Inc. under contract Nol NO1-CP-56019 (5/94;rev. 6/95 - this document has been reformatted from WordPerfect 6.1 to Word (7/95)