Toxicity and Physical Properties of Atrazine and its Degradation Products: A Literature Survey

Kathleen C. Pugh, Ph.D.
Waste Management and Remediation
Environmental Research Center
Muscle Shoals, Alabama

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Toxicity and Physical Properties of Atrazine and its Degradation Products: A Literature Survey

Abstract

The Tennessee Valley Authority's Environmental Research Center has been developing a means of detoxifying atrazine waste waters using TiO_2 photocatalysis. The toxicity and physical properties of atrazine and its degradation products will probably be required information in obtaining permits from the United States Environmental Protection Agency for the demonstration of any photocatalytic treatment of atrazine waste waters. The following report is a literature survey of the toxicological and physical properties of atrazine and its degradation products.

Part 1. Toxicity of Atrazine and its Degradation Products

In the studies reviewed in this report, atrazine was reported to be more toxic than its degradation products. Atrazine has been reported to have higher chronic toxicity than CIAT towards rat endocrine activity. The degradation product CAAT was less toxic than *s*-triazine (the ring system of triazines) towards birds. For phototrophic microorganisms, the order of toxicity from high to low was: atrazine>CIAT>CEAT. The degradation products OIET and CAAT were found to be nontoxic towards most phototrophic microorganism cultures tested. The Microtox test of bacterial toxicity also showed that atrazine was more toxic than its degradation products with the order of toxicity from high to low reported as: atrazine>CEAT>CIAT. The end product of TiO_2 photocatalytic degradation of atrazine is cyanuric acid (OOOT). Atrazine (LD_{50} 3.0 g/kg) is more than twice as toxic as cyanuric acid (LD_{50} 7.7 g/kg). Based on the literature currently available, it appears that any degradation of atrazine results in less toxic products. Complete degradation of atrazine to cyanuric acid, which can be accomplished using TiO_2 photocatalysis, decreases the toxicity of the waste stream to less than half its original toxicity.

Part 2. Physical Properties of Atrazine and its Degradation Products

The physical properties of atrazine and its degradation products reviewed in Part 2 of this report include melting point, molecular weight, vapor pressure, solubility, and pKa's. Sources for UV, IR, and mass spectral data are also reported. The soil half-lives for atrazine, CIAT, and CEAT are compared to the TiO_2 photocatalytic half-lives for the same compounds. (27 pp)

Key Words: atrazine, degradation products, melting point, physical properties, solubility, TiO_2, toxicity, vapor pressure

Introduction

The Tennessee Valley Authority's Environmental Research Center has been the site of research to develop a means of detoxifying atrazine waste waters using TiO_2 photocatalysis.[1] The toxicity and physical properties of atrazine and its degradation products will probably be required information in obtaining permits from the United States Environmental Protection Agency for the demonstration of any photocatalytic treatment process for atrazine waste waters.

The following is a literature survey of the toxicological and physical properties of atrazine and some of its identified and potential degradation products. A number of the degradation products have been identified during atrazine photocatalysis using TiO_2. Others have been identified as atrazine degradation products in other systems and may later be identified as TiO_2 photocatalysis products. The TiO_2 photocatalytic degradation products identified by Pelizetti and coworkers are shown in the degradation mechanism in Figure 1.[2]

The nomenclature system of Cook,[3] Adams,[4] and Hapeman-Somich[5] is used to label compounds: A, amino; C, chloro; E, ethylamino; I, isopropylamino; O, hydroxy; T, triazine ring. Other abbreviations include D, acetamido, and M, methoxy.

This report is separated into two parts. Part 1 reports literature information on the toxicity of atrazine and its degradation products. Information was not available for some degradation products. This may be due to the fact that certain degradation products have not yet been assigned Chemical Abstracts Service (CAS) Registry Numbers. The Registry of Toxic Effects of Chemical Substances (RTECS) was also searched for data on atrazine and its degradation products. For those compounds for which data could be obtained, the LD_{50} (lethal dose for 50% of test subjects, usually rats or mice) is given when reported. Other available toxicological information is also reviewed in Part 1.

Part 2 of this report summarizes the physical properties of atrazine and its degradation products. These properties include melting point, molecular weight, vapor pressure, solubility data, pKas and soil metabolism rates when available.

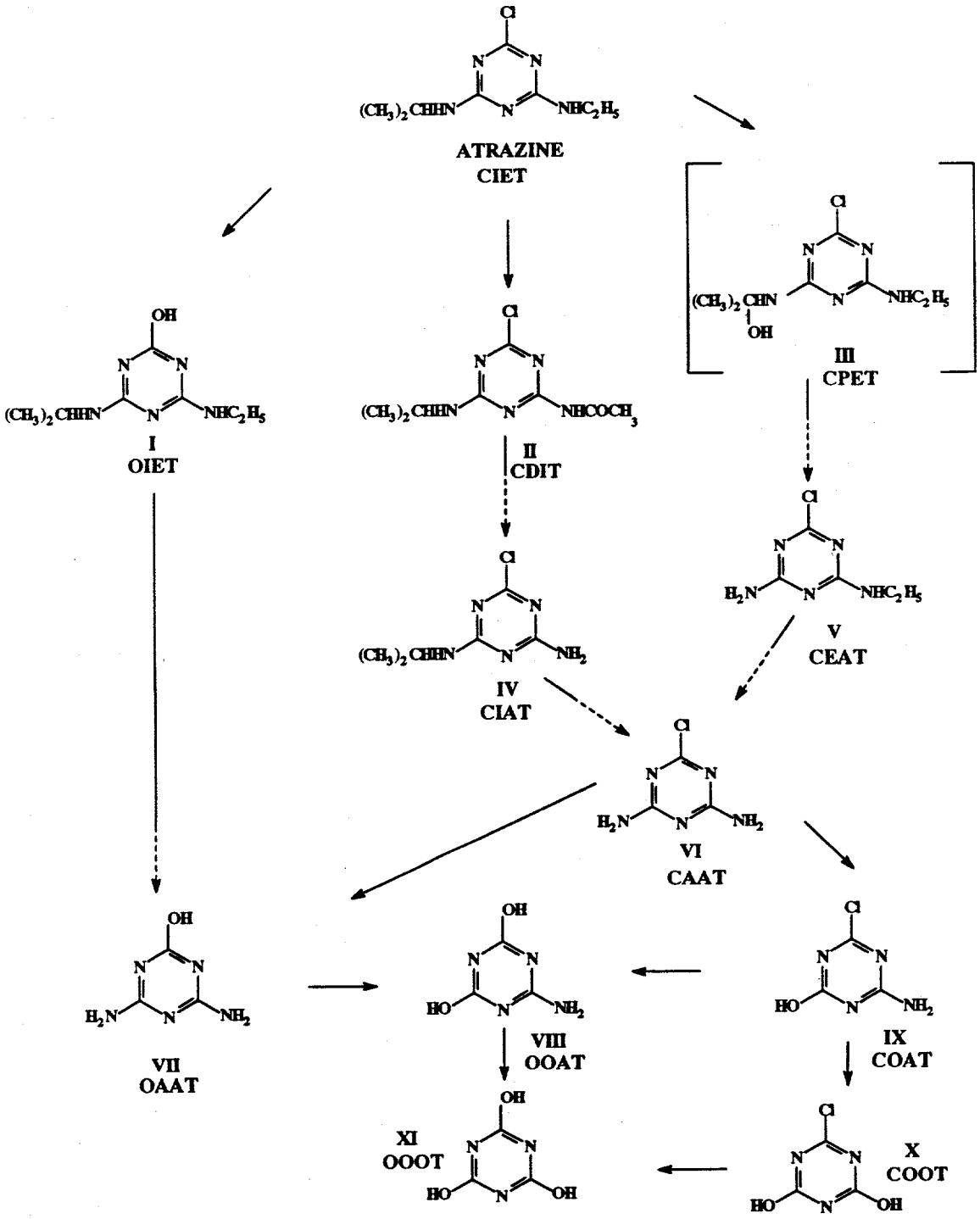


Figure 1. TiO_2 Photocatalytic Degradation of Atrazine Proposed by Pelizzetti and Coworkers.[2]

Part 1: Toxicity of Atrazine and its Degradation Products

For the purpose of providing background information for an audience less familiar with toxicology, Table I gives commonly accepted classifications of toxicity ratings. To put these classifications into perspective, Table II lists the Lethal Dose for 50% of Subjects (LD_{50}) for some well known chemicals. These charts were provided by the PACS consulting firm, courtesy of Dr. Henry Nowicki.[6]

Toxicity data for atrazine and cyanuric acid was relatively abundant. However, little or no data was available for most of the degradation products. In some cases, the CAS Registry number has not yet been assigned to the degradation product, so a computer search was not possible. A search by chemical name was difficult because the nomenclature for atrazine derivatives varies from paper to paper.

Some of the studies reviewed here reported the toxicity of a degradation product in a non-mammalian test and therefore no LD_{50} was established for many of the atrazine degradation products. Table III is a compilation of the compound name, its four letter acronym, any known synonyms, its structure, CAS Registry Number, RTECS Number, and LD_{50} for the cases in which data was available.

Table I. Toxicity Rating Chart[6]

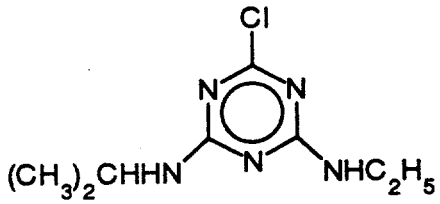
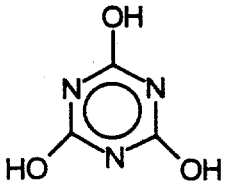
Toxicity rating or class	Probable oral lethal dose for humans, mg/kg [a]
Practically nontoxic	>15,000
Slightly toxic	5,000-15,000
Moderately toxic	500-5000
Very toxic	50-500
Extremely toxic	5-50
Super-toxic	<5

[a]Indicates lethal dose for 50% of subjects.

Table II. Approximate Oral Acute LD_{50}s in Rodents

Agent	LD_{50} (mg/kg)
Sodium chloride (table salt)	4,000
Ferrous sulfate (prescribed for anemia)	1,520
2,4-D (a weed killer)	368
DDT (an insecticide no longer used)	135
Caffeine (in coffee)	127
Nicotine (in tobacco)	24
Strychnine sulfate (used to kill pests)	3
Botulinus toxin (in spoiled food)	0.01

Table III. Atrazine and Degradation Products

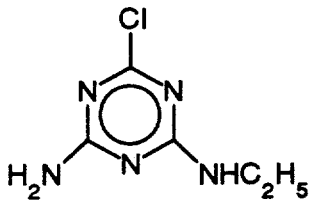
Name(s)	Structure	LD_{50} (mg/kg)
Atrazine		
CIET (2-Chloro-4-ethylamino-6-isopropylamino-*s*-triazine) (6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine) Aatrex, Gesaprim, G30027, Atratol		
CAS No. 1912-24-9 RTECS No. XY5600000		1750, oral, mouse[7] 3000, oral, rat[7]
Cyanuric Acid		
OOOT (Isocyanuric acid) (2,4,6-Trihydroxy-*s*-triazine)		
CAS No. 108-80-5 RTECS No. XZ1800000		3400, oral, mouse[8] 7700, oral, rat[8] >500, ivn,[a] mouse[8] >100, ivn, rat[8]

[a]Intravenous administration.

Table III (continued). Atrazine and Degradation Products

Name(s)	Structure	LD_{50} (mg/kg)

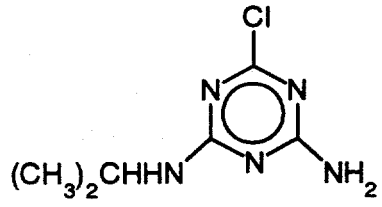
Atrazine desisopropyl



CEAT
(2-Amino-4-chloro-6-ethylamino-*s*-triazine)
(6-Chloro-N-ethyl-1,3,5-triazine-2,4-diamine)
(2,4-Diamino-6-chloro-N-ethyl-1,3,5-triazine)

CAS No. 1007-28-9
RTECS No. unknown

Atrazine desethyl



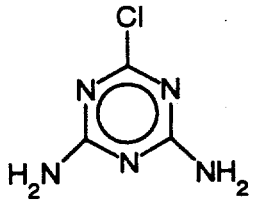
CIAT
(2-Amino-4-chloro-6-isopropylamino-*s*-triazine)
(4-Amino-2-chloro-6-isopropylamino-s-triazine)
(6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine)
(2,4-Diamino-6-chloro-N-(1-methylethyl)-1,3,5-triazine)

CAS No. 6190-65-4
RTECS No. unknown

Table III (continued). Atrazine and Degradation Products

Name(s)	Structure	LD_{50} (mg/kg)

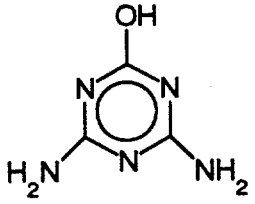
2-chloro-4,6-diamino-*s*-triazine



CAAT
(Didealkylatedatrazine)
(2,4-Diamino-6-chloro-1,3,5-triazine)

CAS No. 3397-62-4
RTECS No. unknown

Ammeline



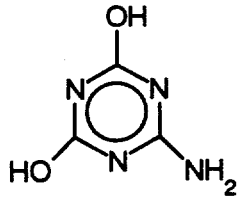
OAAT
(2,4-Diamino-6-hydroxy-s-triazine)
(Atrazine desethyl desisopropyl-2-hydroxy)
(4,6-Diamino-1,3,5-triazine-2(1H)-one)
[*s*-Triazin-2-ol, 4,6-diamino-(8CI)]
[1,3,5-Triazin-2(1H)-one, 4,6-diamino-(9CI)]

CAS No. 645-92-1
RTECS No. unknown

Table III (continued). Atrazine and Degradation Products

Name(s)	Structure	LD_{50} (mg/kg)

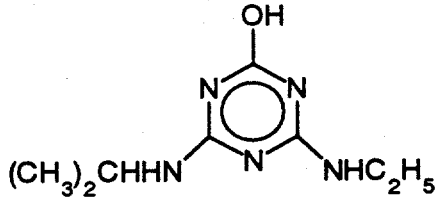
Ammelide[9]



OOAT
(2-Amino-4,6-dihydroxy-*s*-triazine)
(6-Amino-1,3,5-triazine-2,4(1H,3H)-dione)
(1,3,5-Triazine-2,4(1H,3H)-dione, 6-amino-)

CAS No. 645-93-2
RTECS No. unknown

Hydroxyatrazine



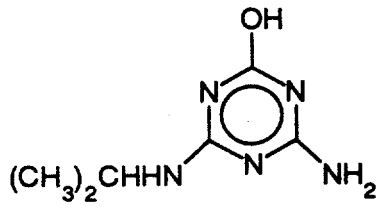
OIET
(Atrazine-2-hydroxy)
(4-(Ethylamino)-2-hydroxy-6-isopropylamino-*s*-triazine)
(2-Hydroxy-4-ethylamino-6-isopropylamino-*s*-triazine)
(4-(Ethylamino)-6-[1-methylethyl]amino-1,3,5-triazine-2-(1H)one)
(2-Ethylamino-4-hydroxy-6-isopropylamino-*s*-triazine)
(2,4-Diamino-6-hydroxy-N-ethyl-N'(methylethyl)-1,3,5-triazine)

CAS No. 2163-68-0
RTECS No. unknown

Table III (continued). Atrazine and Degradation Products

Name(s)	Structure	LD_{50} (mg/kg)

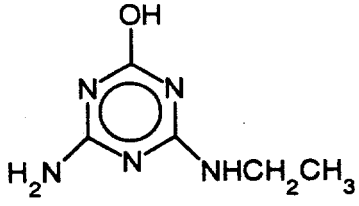
2-Amino-4-hydroxy-6-isopropylamino-*s*-triazine



OAIT
(4-Amino-6-[(1-methylethyl)amino]-1,3,5-triazine-2(1H)-one)
(N-Isopropylammeline)
(Atrazine desethyl-2-hydroxy)
(4-Amino-2-hydroxy-6-isopropylamino-*s*-triazine)

CAS No. unknown
RTECS No. unknown

2-Amino-4-ethylamino-6-hydroxy-*s*-triazine



OAET
(4-Amino-6-(ethylamino)-1,3,5-triazine-2(1H)-one)
(N-ethylammeline)

CAS No. unknown
RTECS No. unknown

Table III (continued). Atrazine and Degradation Products

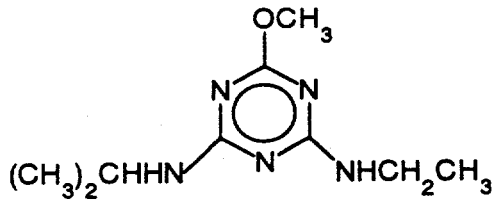
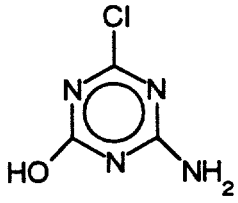
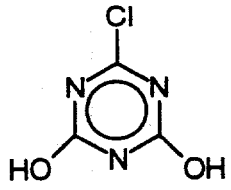
Name(s)	Structure	LD_{50} (mg/kg)
Atraton		
MEIT (2-Methoxy atrazine) (2-[Ethylamino]-4-[isopropylamino]-6-methoxy-*s*-triazine) (Gestamine) CAS No. 1610-17-9 RTECS No. XY8750000		1465, oral, rat or mouse[10]
2-amino-4-chloro-6-hydroxy-*s*-triazine		
COAT CAS No. unknown RTECS No. unknown		

Table III (concluded). Atrazine and Degradation Products

Name(s)	Structure	LD_{50} (mg/kg)

2-chloro-4,6-dihydroxy-*s*-triazine



COOT

CAS No. unknown
RTECS No. unknown

Atrazine

A search of the CAS and Beilstein databases for "atrazine" cross referenced with "toxicity" led to 460 references. The information from only a select few of these references will be presented here.

The Material Safety Data Sheets (MSDS) for atrazine and its degradation products were provided by the suppliers: Aldrich (Milwuakee, WI), Supelco (Bellefonte, PA), Chem Service (West Chester, PA), and Ciba-Geigy, Inc. (Greensboro, NC).

Acute Toxicity

Target organs for atrazine include skin, eyes, mucous membranes, respiratory system, kidneys, and liver.[11,12]

Most MSDSs for atrazine list the LD_{50} (oral, rat or mouse) as 1750 mg/kg. Ciba-Geigy's MSDS reports a LD_{50} of 3090 mg/kg (oral, rat), >3,100 mg/kg (dermal, rat), and a LC_{50} of 1.8 mg/L air 4 hours (inhalation, rat). The *Handbook of Toxic and Hazardous Chemicals, 3rd ed.*,[7] reports a LD_{50} of 1750 mg/kg (oral, mouse) and 3000 mg/kg (oral, rat), but notes that the purity of the compounds in these studies was not specified. The *Registry of Toxic Effects of Chemical Substances* (RTECS) lists a LD_{50} of 672 mg/kg (oral, rat) and 850 mg/kg (oral, mouse) for atrazine,[11] according to a National Toxicology Program report.[12]

Fish Toxicity

An investigation of acute and subacute toxicity of atrazine on Carp (Cyprinus carpio L.) was performed by Neskovic and coworkers.[13] These researchers reported that atrazine is only slightly toxic to Carp according to its LC_{50} , but provokes certain biochemical and histopathological changes in some organs and tissues of fish. The most pronounced effects are on the AP (alkaline phosphatase) activity in the serum and some organs. Cell changes were most pronounced in the gills and the liver.

Chronic Toxicity

The chronic toxicity of atrazine was discussed in Ciba-Geigy's MSDS. Atrazine has been shown to cause an increased incidence of mammary tumors in female Sprague-Dawley rats during long-term feeding studies. Atrazine also causes cardiotoxicity in dogs and mice. According to Ciba-Geigy, some studies which showed mutagenic effects of atrazine on barley seeds and corn plants were later successfully refuted (no references). However, a National Toxicology Report,[12] referring to the RTECS entry for atrazine,[11] lists atrazine as a mutagen, tumorigen, and reproductive abnormality inducer.

The *Handbook of Toxic and Hazardous Chemicals, 3rd ed.*,[7] reported that toxicity data on atrazine were reviewed by the National Academy of Sciences and were used to identify a chronic NOAEL (No Adverse Effects Level) of 21.5 mg/kg/day. Although at that time it was concluded that atrazine has low chronic toxicity, an uncertainty factor of 1,000 was employed in calculation of the ADI (acceptable daily intake) since only limited data were available. The resulting value

(0.021 mg/kg/day) corresponds to an ADI of 0.73 mg/L in a 70-kg adult consuming 2 L of water per day.

Cyanuric Acid (OOOT)

Acute toxicity

Unlike atrazine, cyanuric acid (OOOT) is practically nontoxic when administered as a single oral or dermal dose.[14] Hammond and coworkers reported a LD_{50} (oral, rat) of >10 g/kg,[14] but an earlier report sited the LD_{50} (oral, rat) as >5.00 g/kg.[15] The RTECS entry for OOOT listed the LD_{50} (oral, rat) as 7.7 g/kg and the LD_{50} (oral, mouse) as 3.4 g/kg. The dermal rabbit LD_{50} for OOOT was reported as >7.94 g/kg.[14] The Federal Hazardous Substances Act Test (rabbit, eye) was 1.5/110, which led to the classification of OOOT as a slight irritant. OOOT has been shown to be poorly absorbed when applied dermally.[16] OOOT is very toxic towards certain types of barley and radishes.[17]

Chronic Toxicity

The chronic toxic effects of OOOT were reviewed by Canelli in 1974.[18] At a dose of 30 mg/kg/day, dystrophic changes in the kidneys of guinea pigs and rats were observed. However, at a lower dose of 10 mg/kg/day, no changes in kidney tissue were observed.[15,19]

Carcinogenic Effects

A low blastomogenic effect in rats and mice (tumors after 18 months) due to administration of OOOT has been reported, but adequate controls were not part of this study and benzene and oil were used to administer some doses.[20] The RTECS entry for OOOT gave the status of "equivocal tumorigenic agent" for all RTECS criteria.[11]

Metabolism

OOOT has been shown to be readily eliminated from the body unchanged.[14] Studies in which rats were given both oral and intravenous administration of OOOT demonstrated that OOOT is excreted, primarily in urine, unchanged.[21] No bioaccumulation of radiolabeled OOOT was observed.

Atraton (MEIT)

Although atraton (MEIT) is not one of the degradation products generated during TiO_2 photocatalysis of atrazine,[22] it is a common soil metabolite of atrazine. A LD_{50} of 1465 mg/kg (oral, rat) for this compound was reported on the Chem Service, Inc. MSDS. The RTECS entry for MEIT listed a LD_{50} (oral, rat) of 1465 mg/kg and a LD_{50} (oral, mouse) of 905 mg/kg. Several studies have been done to try to predict the relative toxicity of atraton using quantitative

structure-activity relationships (QSAR's).[23] Because the data in these studies has not been experimentally verified, it will not be presented here.

Comparison of Toxicities

Although there is an abundance of mammalian toxicity data on atrazine and cyanuric acid, many of the other degradation products of atrazine have no mammalian toxicological data. One exception is a study which compared the toxicity of atrazine to one of its degradation products, CIAT, in the endocrine system of rats.[24] The gonadotropic systems of rat offspring were found to develop more slowly when mother rats were treated with atrazine during pregnancy and lactation. These observations were the result of alteration of 5-alpha-R activity in the anterior of the pituitary gland and inhibition of the 5-alpha-DHT prostate receptor. CIAT also influenced activities of hormones in the anterior of the pituitary gland, and significantly increased the weight of the gland. However, the researchers concluded that the parent compound, atrazine, exhibited more significant chronic effects than did CIAT.[24, 25]

Despite the paucity of studies comparing the toxicity of atrazine and its degradation products in mammalian systems, such studies have been carried out using species other than mammals. The toxicity of atrazine and its degradation products was compared in studies using domestic and wild birds,[26] phototropic microorganisms,[27] bacteria (Microtox), [28] and certain plants.[29] Summaries of those studies follows.

Avian Toxicity

An evaluation of 998 chemicals for avian toxicity, stupefaction, and/or repellency was conducted by the Wildlife Research Center in Denver, CO.[26] Included in the study were the chemicals *s*-triazine (the basic ring system for triazine pesticides, including atrazine) and CAAT. The relevant data are summarized in Table IV.

Table IV.[a] Relevant Data for Avian Toxicity and Repellancy[26]

Name	Registry number (CAS)	LD_{50} (mg/kg)	Redwinged blackbird R_{50}	R_{50} (mg/kg)	Hazard factor[b]	Starling LD_{50} (mg/kg)	Coturnix LD_{50} (mg/kg)
s-Triazine	290879	100	>1.00	>76.9	<0.769	----	237
CAAT	3397624[c]	>100	>1.00	----	----	----	>316

[a]The data in Table IV were chosen from data in Reference 26.
[b]Calculated by dividing the R_{50} (maximum value) by the LD_{50}.
[c]Mistakenly listed in Reference 26 as 3797624.

The "Hazard Factor" listed in Table IV is a repellency-toxicity index and was calculated by assuming that at a R_{50} (i.e., concentration at which 50% of the birds were repelled), a bird would eat half of its maximum food intake. The amount of food a bird would eat at 50% repellency (in mg/kg) was then when divided by the LD_{50} (in mg/kg), to provide an index for likelihood of acute oral poisoning in the wild. An index value of >1.00 indicates well-accepted toxic agents which have definite potential for causing acute poisoning episodes.

The data in Table IV show that the basic *s*-triazine ring structure has a lower general LD_{50} than CAAT. This indicates that CAAT is less acutely toxic than the *s*-triazine ring structure towards birds. The LD_{50} of CAAT was also higher than that of the *s*-triazine ring for one particular species, Coturnix. Unfortunately, not enough data was available to compare the hazard factors for CAAT and the triazine ring system. However, the triazine ring system was determined to have a hazard factor of <0.769, indicating possible potential for causing acute poisoning episodes in the wild.

Microorganism Toxicity

In another study entitled "Effects of the Herbicide Atrazine and its Degradation Products, Alone and in Combination, on Phototrophic Microorganisms,"[27] the toxicity of atrazine, CEAT, CIAT, CAAT, and OIET towards phototrophic microorganisms was examined. The author evaluated the toxic effects of the above-mentioned compounds for growth, photosynthesis, and nitrogenase activity (acetylene-reducing ability) of two species of green and three species of cyanobacteria. Atrazine was significantly more toxic than its degradation products toward the above test criteria. Table V contains a summary of the data from this paper. In general, the toxicities were: atrazine>CIAT>CEAT. The compounds OIET and CAAT were found to be nontoxic towards most of the cultures tested.

Table V. Summary of Toxicity Data for *s*-Triazines Toward Phototrophic Microorganisms[27]

Name	EC_{50} (ppm or ug/mL)[a]	Test
Atrazine	0.1-0.5	Photosynthesis
	0.03-5.0	Growth
	55 +/- 15	Acetylene Reduction[b]
CIAT	0.7-4.8	Photosynthesis
	1.0-8.5	Growth
CEAT	3.6-9.3	Photosynthesis
	2.5->10	Growth
OIET	nontoxic	Photosynthesis, growth
CAAT	nontoxic	Photosynthesis, growth

[a]The term EC_{50} refers to the effective concentration which elicits a 50% inhibition of the test parameter in question, calculated with reference to activity in appropriate control systems.
[b]For cyanobacteria only atrazine had an effect. Cyanobacteria were insensitive to the other compounds.

Bacterial Toxicity

The Microtox method of toxicity assessment was performed on atrazine and two of its environmental metabolites: CIAT and CEAT.[28] Microtox is a system manufactured by Microbics Corporation which utilizes a photomultiplier tube to measure light from bioluminescent bacteria. Although the mechanism of toxicity is not determined by this test, a relative assessment of toxicity is determined by measuring inhibition of light production by certain microorganisms. The study showed that CIAT and CEAT were less toxic than their parent compound, atrazine. The relevant data from this study are summarized in Table VI.

Table VI. Summary of Toxicities Toward Bioluminescent Bacteria as Determined by Microtox[28]

Name	Time (min)	EC_{10}[a]	EC_{20}[a]	EC_{50}[a]
Atrazine	5	13.0	25.8	95[b]
	15	14.4	22.6	~40[b]
	30	17.5	24.0	~25[b]
CEAT	5	44.0	107.0	~400[b]
	15	63.0	109.0	~305[b]
	30	75.0	116.0	~290[b]
CIAT	5	70.0	180.0	~700[b]
	15	101.0	193.0	~580[b]
	30	134.0	220.0	~580[b]

[a]ECx is the effective concentration at which light produced by the bacteria is reduced by x percentage.
[b]Values were read from a graph and are not necessarily accurate.

The low toxicities of atrazine, CIAT, and CEAT toward the bacteria in question led the researchers to report EC_{10} and EC_{20} values in addition to the usual EC_{50} value. This was because EC_{10} and EC_{20} concentrations were much closer to possible environmental concentrations of the chemicals under study. The general order of toxicities was: atrazine>CEAT>CIAT. The toxicity of atrazine remained stable over time, whereas the toxicities of CEAT and CIAT decreased over longer testing times.[28]

Plant Toxicity

Crops such as corn, sorghum, and sugar cane are tolerant of atrazine, a broad-leaf herbicide, because they are able to biochemically degrade the herbicide to its nontoxic metabolites.[30] The toxicity of atrazine and its metabolites were compared in one plant study. Dealkylation products, such as CIAT and CEAT, were found to remain somewhat toxic.[29] In another study of a fungus (Cochliobolus Sativus), atrazine inhibited germination of conidia, but OIET was found to act as a germination stimulant, possibly even lethally over stimulating the organisms.[31] The authors of the fungus study report previously unpublished data which suggest that several common degradation products of atrazine (other than OIET) inhibit germination of the conidia, but the degradation products are not identified specifically.

Conclusions

In the studies reviewed in this report, in general, atrazine was reported to be more toxic than its degradation products. Atrazine has been reported to have higher chronic toxicity than CIAT towards rat endocrine activity. The degradation product CAAT was less toxic than the *s*-triazine ring towards birds. For phototrophic microorganisms, the order of toxicity from high to low was: atrazine> CIAT>CEAT. The degradation products OIET and CAAT were found to be nontoxic towards most phototrophic microorganism cultures tested. The Microtox test of bacterial toxicity also showed that atrazine was more toxic than its degradation products with the order of toxicity from high to low reported as: atrazine>CEAT>CIAT.

Of particular interest for the TiO_2 photocatalytic project is a comparison of the toxicity of the starting compound, atrazine, with the final degradation product, cyanuric acid (OOOT). Mammalian LD_{50}'s for both of these compounds have been established. Atrazine (LD_{50} 3.0 g/kg) is more than twice as toxic as cyanuric acid (LD_{50} 7.7 g/kg).

In conclusion, based on the literature currently available, it appears that any degradation of atrazine results in less toxic products. Complete degradation of atrazine to cyanuric acid, which can be accomplished using TiO_2 photocatalysis, decreases the toxicity of the waste stream to less than half its original toxicity.

Whereas atrazine is considered to be moderately toxic, cyanuric acid has been classified as practically nontoxic by Hammond and coworkers. The degradation of atrazine to cyanuric acid would, therefore, represent a significant toxicological risk reduction for atrazine-contaminated waters.

Part 2: Physical Properties of Atrazine and Its Degradation Products

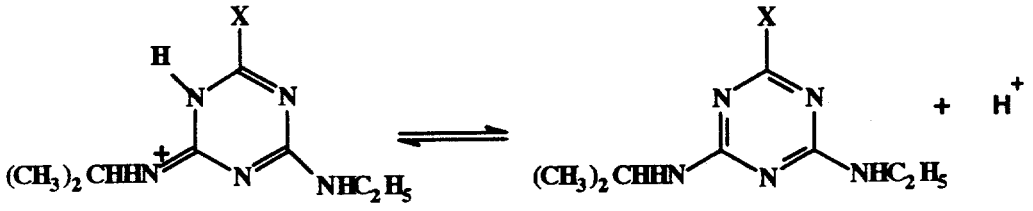
The physical properties of atrazine and its degradation products which will be discussed in this section include melting point, molecular weight, vapor pressure, solubility, and pKa's. Sources for UV, IR, and mass spectral data are reported. The soil half-lives for atrazine, CIAT, and CEAT are compared to the TiO_2 photocatalytic half-lives for the same compounds.

Melting Point and Molecular Weight

The melting point and molecular weight of atrazine and thirteen degradation products are shown in Table VII.

Vapor pressure and solubilities of atrazine and nine of its degradation products are given in Table VIII.

In Table IX, the pKa's of atrazine and its degradation products are shown. A schematic of the dissociation in question is shown below:[41]



If X = Cl, pKa = ~2
If X = OH, pKa = ~5

A comparison of the soil half-lives and TiO_2 photocatalytic half-lives for atrazine, CIAT, and CEAT are given in Table XI. This data was included to give a comparison of the degradation rates for atrazine with the degradation rates of its intermediates by TiO_2 photocatalysis.[22] The predominant soil metabolite of atrazine was found to be CIAT.[55] CIAT was also found to be more mobile in soils than atrazine whereas CEAT was found to have about the same soil mobility as atrazine.[27,28] The soil degradation of atrazine is greatly influenced by low pH, mineral salts, organic matter and photolysis.[32]

Table VII. Melting Point and Molecular Weight of Atrazine and Thirteen of Its Degradation Products

Compound	Melting point (°C)	Molecular weight
1. Atrazine	175-177[b,d]	215.7
2. OOOT	>360[a]	129.1
3. CEAT	164-166[b] or 177-179[c]	173.6
4. CIAT	132-134[d] or 42-50[b]	187.6
5. OIAT	>310[b]	169.2
6. CAAT	320[d]	145.6
7. OAAT	>320	127.1
8. OOAT	NA	128.1
9. OIET	>310[d] or >250[e]	197.2
10. CDAT	225 (dec.)[f]	187.6
11. CDIT	177-178[f] or 187-188[g]	229.7
12. CDET	180-181[f]	215.6
13. CDDT	197-198[f]	229.6
14. COAT	NA	146.5
15. COOT	NA	147.5
16. MEIT	95-96[d]	211.3

NA: Not Available
[a]The Merck Index reports that cyanuric acid does not melt, it evolves cyanic acid on heating.[17]
[b]From Ciba-Geigy MSDS
[c]See Reference 33
[d]From Chem Service, Inc. MSDS
[e]Reference 34 reports OIET decomposes without melting at >250 °C
[f]See Reference 5
[g]See Reference 35

Table VIII. Vapor Pressure and Solubility of Atrazine and Nine of Its Degradation Products

Compound	Vapor pressure (mm Hg)	Solubility
1. Atrazine	6.6×10^{-7} (at 25 °C)[a] 3×10^{-7} (at 20 °C)[b,c]	33 ppm/H_2O/22 °C[a,e,f] 31 ppm/pH 3.0[g] 34.7 ppm/pH 7.0[g] 36.7 ppm/pH 10.0[g] 1800 ppm/MeOH/27 °C 52 ppm/$CHCl_3$/27 °C >6470 ppm/EtOH
2. OOOT	NA	2600 ppm/H_2O[d] 2967 ppm/H_2O[e] 3200 ppm/MeOH[d] 6000 ppm/THF[d] 10,200 ppm/1,4-Dioxane[d]
3. CEAT	NA	>114 ppm/H_2O >1533 ppm/MeOH
4. CIAT	NA	>~438 ppm/H_2O 375 ppm/H_2O[e] >5867 ppm/MeOH
5. OIAT	3×10^{-7} (at 20 °C)[b]	NA
6. CAAT	NA	NA
7. OAAT	3×10^{-7} (at 20 °C)[b]	76.2 ppm/H_2O[e] 762 ppm/0.1 M HCl
8. OOAT	NA	76.8 ppm/H_2O[e] 1280 ppm/0.1 M NaOH
9. OIET	NA	47.3 ppm/H_2O[e]

NA: not available
[a]Ciba-Geigy MSDS
[b]Chem Service MSDS
[c]See Reference 36; the data was converted from Pa to mm Hg.
[d]See Reference 37
[e]See Reference 38
[f]See Reference 39
[g]See Reference 40

Table IX. pKa's for Atrazine and Its Derivatives

Compound	pKa^1	pKa^2
1. Atrazine	1.71[a] 1.85[b] 1.68[c]	
2. OOOT[e]	6.51[d]	10.60[d]
3. CEAT	1.58[a]	
4. CIAT	1.65[a]	
5. OIAT[e]	4.57[a]	
6. OEAT[e]	4.65[a]	
7. CAAT		
8. OAAT[e]		
9. OOAT[e]		
10. OIET[e]	5.15[a] 5.20[b]	
11. COAT[e]		
12. COOT[e]		

[a]See Reference 41
[b]See Reference 42
[c]See Reference 43
[d]See Reference 37
[e]The dissociation constant for the hydroxy group on the hydroxyatrazines is about 11.[41]

Table X. UV, IR, and Mass Spec Data Sources

Compound	UV	IR	Mass spec
1. Atrazine	41	44	
2. OOOT	45	46,47,48,49	
3. CEAT	41	50,51	52
4. CIAT	41	50	
5. OIAT	41		
6. OEAT	41		
7. CAAT		49, 53	52
8. OAAT	54	49	47
9. OOAT		47, 49	

Table XI. Half-Lives for Atrazine and Its Degradation Products in Soil and During TiO_2 Photocatalysis

Name	TiO_2 half life	Reference	Soil half-life	Reference
Atrazine	4 hours	22	0.5-6 months	55
CEAT	4.8 hours	22	5 months	27
CIAT	6 hours	22	>5 months	27

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