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Excerpts from Verschueren, K., 2001. *Handbook of Environmental Data on Organic Chemicals*, 4th ed., John Wiley & Sons, Inc., New York, New York. http://www.knovel.com/knovel2/ (Verschueren 2001, 90563)

Chemical Name	Original page numbers in reference
Alachlor	133-135
Aroclor-1016	224
Aroclor-1221	224-225
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Dinitrobenzene[1,3-] (meta)	953-954
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Dinitrotoluene[2,3-]	967-968
Dinitrotoluene[2,4-]	968-970
Dinitrotoluene[2,5-]	970-971
Dinitrotoluene[2,6-]	971-972
Dinitrotoluene[3,4-]	972-973
Dinitrotoluene[3,5-]	973
Glyphosate	1202-1204
Heptachlor Epoxide	1214-1215
Methyl tert-Butyl Ether (MTBE)	1467-1468
Naphthalene	1575-1580
Nitrobenzene	1612-1614
Tetrachloroethane[1,1,1,2-]	1948
Tetrachloroethane[1,1,2,2-]	1946-1947
Trichlorobenzene[1,2,3-]	2044-2047
Trichlorobenzene[1,2,4-]	2047-2051
Trichlorobenzene[1,3,5-]	2051-2052
Trinitrobenzene[1,3,5-]	2142-2143
Trinitrotoluene[2,4,6-]	2144-2149

14623

Handbook of Environmental Data on Organic Chemicals

Fourth Edition

VOLUME 1

Karel Verschueren
President
Verschueren Environmental Consultancy

Series in Conjunction with Environmental Protection Magazine
Dallas, Texas

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For ordering and customer service, call 1-800-CALL-WILEY.

Library of Congress Cataloging-in-Publication Data:

Verschueren, Karel, 1944–
Handbook of environmental data on organic chemicals / Karel Verschueren—4th ed.
p. cm
Includes index.
ISBN 0-471-37490-3 (cloth: alk. paper)
1. Organic compounds–Environmental aspects–Handbooks, manuals, etc. I. Title.

TD196.O73 V47 2001
363.738–dc21

00-069254

Printed in the United States of America.

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CAS CROSS-INDEX 2377

apor pressure 2

(41)

ved

(93)

(41)

(41)
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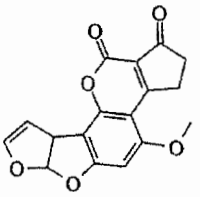
of toxicant con-
ish: 68 h in soft

water at 22–24.5°C. (474)

aflatoxin B1



aflatoxin B1

$C_{17}H_{12}O_6$

CAS 1162-65-8

OCCURRENCE: belongs to a group of polynuclear molds (mycotoxins) produced chiefly by the fungus *Aspergillus flavus;* natural contaminants of a wide range of fruits, vegetables, and cereal grains.

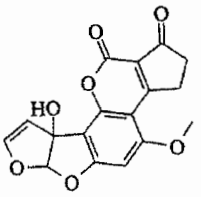
A. PROPERTIES: a crystalline material; molecular weight 312.29; melting point 268°C.

B. AIR POLLUTION FACTORS:

Incinerability: thermal stability ranking of hazardous organic compounds: rank 200 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

D. BIOLOGICAL EFFECTS:

Confirmed human carcinogen with experimental tumorigenic, neoplastigenic, and carcinogenic data. Aflatoxin B1 is oxidized by mammals to aflatoxin M1, which is also a confirmed carcinogen with experimental tumorigenic data.

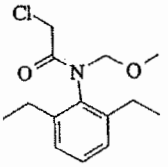


aflatoxin M1

(3998)

AGE *see* allylglycidylether

alachlor (2-chloro-2';6';-diethyl-N-(methoxymethyl)acetanilide)



$(CH_3CH_2)_2C_6H_3N(CH_2OCH_3)COCH_2Cl$

$C_{14}H_{20}ClNO_2$

134 alachlor

CAS 15972-60-8

USES: a selective herbicide used to control annual grasses and many broad-leaved weeds in cotton, brassicas, maize, oilseed rape, peanuts, radish, soybeans, and sugarcane.

A. PROPERTIES: colorless to yellow crystals; molecular weight 269.77; melting point 40°C; boiling point decomposes at 105°C; vapor pressure 2.9 x 10^{-5} hPa at 20°C; d 1.13 at 20°C; solubility 148 mg/L at 20°C, 240 mg/L; log P_{oct} 2.8.

C. WATER AND SOIL POLLUTION FACTORS:

Water treatment:

initial concentration, µg/L	*treatment method*	*% removal*	
7	flocc. + sedim. + filtr. + chlorination	24	
4	chlorination + filtration	15	
1.4	chlorination	1	
1.0	chlorination	9	
3.6	flocc. + sedim. + carbonate removal	–5 (increase!)	
not reported	activated carbon	43	(2915)

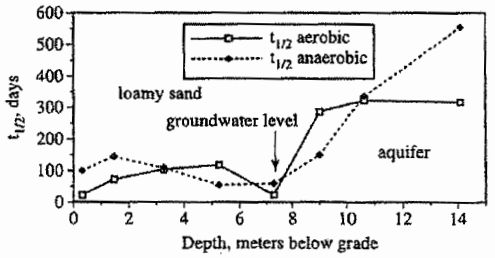
In groundwater wells in the U.S.A.—150 investigations up to 1988:

median of the conc.'s of positive detections for all studies	0.9 µg/L	
maximum conc.	113 µg/L	(2944)

Degradation in soil (see also graph): degradation in soils (Eustis loamy sand) and the underlying vadose zone and aquifer materials: half-life ($t_{1/2}$) at 20°C:

soil depth, m	*under aerobic conditions* $t_{1/2}$, *d*	*under anaerobic conditions* $t_{1/2}$, *d*	
0.0–0.6	23	100	
Vadose zone			
0.6–2.4	73	144	
2.4–4.3	104	110	
4.3–6.3	116	53	
6.3–8.3	22	57	
8.3–9.6	285	148	
Aquifer			
9.6–11.6	324	337	
13.1–15.2	320	553	(2577)

Alachlor: Half-life in Soil



In soil and in plants, the chlorine atom is rapidly cleaved. Further breakdown to the aniline derivative occurs. After 4–5 weeks in soil, the bulk of applied alachlor is degraded. (2962)

Biodegradation half life time in soil in greenhouse at 23-26°C at constant light at initial conc. of 5-10 mg/kg soil, experiment time 50 d

	t/2 d	
in sandy soil	63	
in organic rich orchard soil	8	
in agricultural soil	13	
in soil from volcanic area	15	
in field experiments	15 (dissipation t/2)	(7045)

Mobility: log K_{oc}: 2.2 (7045)

D. BIOLOGICAL EFFECTS:

Nitrification inhibition in soil (1% organic carbon) after 14 d: 100% at 50 mg/kg. (7050)

alamine 336 (aliphatic amines, C_{12}–C_{18})

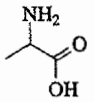
Alamine is a trademark for a series of primary, secondary, and tertiary aliphatic amines, organic substituted ammonia derivatives, chain length from C_{12} to C_{18}, with varying degrees of unsaturation. (1590)

USES: corrosion inhibitors, ore flotation agents, textile finishing agents, rubber compounding. (1590)

D. BIOLOGICAL EFFECTS:

FISHES: rainbow trout: 96h LC_{50}, S: 7.5–10 mg/L (1500)

DL-alanine (DL-2-aminopropanoic acid; DL-α-aminopropanoic acid)



$CH_3CH(NH_2)COOH$

$C_3H_7NO_2$

CAS 302-72-7

A. PROPERTIES: molecular weight 89.09; melting point 295°C; boiling point 200°C sublimes; solubility 166,000 mg/L at 25°C, 322,000 mg/L at 75°C; THC 388 kcal/mole.

C. WATER AND SOIL POLLUTION FACTORS:

BOD_5: 87% ThOD

COD: 77% ThOD (0.05 n K_2CrO_7) (274)

ThOD: 1.08 (30)

Natural sources: in soil: silty loam: 6 to 160 µg/kg soil, (n.s.i.): clay soils: 30 to 400 µg/kg soil

Manmade sources: excreted by humans in urine: 0.55 mg/kg body wt/d; in domestic sewage effluent: 5 µg/L

Waste water treatment:
A.S.

	α-DL-alanine	*β-alanine*	
after 6 h:	12% of ThOD	1.7% ThOD	
12 h:	27% of ThOD	6.9% ThOD	
24 h:	43% of ThOD	16% ThOD	(89)

methods	*temp., °C*	*days observed*	*feed, mg/L*	*days acclim.*	*% theor. oxidation*	*% removed*
A.S., BOD	20	1–5	333	15	–	97
A.S., Resp, BOD	20	1–5	500	>1	39	96

(93)

powdered carbon: at 100 mg/L, carbon dosage 1,000 mg/L: 1% absorbed (n.s.i.) (520)

alar (succinic acid, 2,2-dimethylhydrazide; aminoazide)

$C_6H_{12}N_2O_3$

CAS 1596-84-5

Biodegradation half-lives in nonadapted aerobic subsoil: groundwater Ohio: 0.03–0.17 d. (2695)

D. BIOLOGICAL EFFECTS:

Toxicity to microorganisms: nitrification inhib. EC_{50}: 1.7 mg/L (L-arginine). (2624)

aroclor 1016 *see* also polychlorobiphenyls. A mixture of polychlorobiphenyls containing on average 16 wt % of chlorine.

A. PROPERTIES: solubility 0.22–0.25 mg/L; 0.049 mg/L at 24°C.

Composition of the water soluble fraction (WSF)				
monochloro isomers	111 µg/L	or	12% of WSF	
dichloro isomers	280 µg/L	or	31% of WSF	
trichloro isomers	329 µg/L	or	36% of WSF	
tetrachloro isomers	186 µg/L	or	21% of WSF	
total WSF	906 µg/L		100%	(1909)

C. WATER POLLUTION FACTORS: Partition coefficients to natural sediments.

sediment	*% organic carbon*	*partition coefficient*
Oconee River	0.4	620
USDA Pond	0.8	1,370
Doe Run Pond	1.4	1,290
Hickory Hill Pond	2.4	1,300

D. BIOLOGICAL EFFECTS: Concentration of aroclor 1016 in fish confined to a live-cage for 14 d near Rodger's Island in the Hudson River: average conc. of aroclor 1016 in Hudson water: 0.17 µg/L.

	µg/kg whole fish	*BCF*	
creek chubsucker *(Ermyzon oblongus)*	2,200	13,000	
yellow perch *(Perca flavescens)*	1,800	10,600	
pumpkinseed *(Lepomis gibbosus)*	2,500	14,700	
brown bullhead *(Ictalurus nebulosus)*	3,800	22,300	
	2,800	17,000	(1434)

aroclor 1221 *see* also polychlorobiphenyls. A mixture of polychlorobiphenyls containing on average 21 wt % of chlorine.

CAS 11104-28-2

A. PROPERTIES: solubility 0.59 mg/L at 24°C.

Composition of the water soluble fraction (WSF)				
monochloro isomers	3,241 µg/L	or	92% of WSF	
dichloro isomers	233 µg/L	or	7% of WSF	
trichloro isomers	31 µg/L	or	1% of WSF	
tetrachloro isomers	11 µg/L	or	0.3% of WSF	
total WSF	3,516 µg/L	or	100%	(1909)

C. WATER POLLUTION FACTORS:

Biodegradation at 0.1 mg/L	normal sewage	adapted sewage	
after 24 h	0%	49%	
after 135 h	12%	96%	(997)

D. BIOLOGICAL EFFECTS:

(2695)

FISHES: harlequin fish *(Rasbora heteromorpha):*

mg/L	*24 h*	*48 h*	*96 h*	
LC_{10}	1.1	1.05	0.98	
LC_{50}	1.3	1.15	1.05	(331)

cutthroat trout: 96h LC_{50} 1.2 mg/L (1617)

(2624)

aroclor 1232

6 wt % of chlorine.

CAS 11141-16-5

D. BIOLOGICAL EFFECTS:

FISHES: harlequin fish *(Rasbora heteromorpha)*

mg/L	*24 h*	*48 h*	*96 h*	
LC_{10}	0.52	0.27	–	
LC_{50}	0.9	0.56	0.32	(331)

cutthroat trout: 96h LC_{50} 2.5 mg/L (1617)

(1909)

aroclor 1242

CAS 53469-21-9

USES AND FORMULATIONS: dielectric liquids; thermostatic fluids; swelling agents for transmission seals; additives or bases for lubricants, oils, and greases; plasticizers for cellulosics, vinyls, and chlorinated rubbers. A mixture of polychlorobiphenyls containing an average of 42 wt % chlorine.

A. PROPERTIES: vapor pressure 50 mm at 225°C; d 1.41 at 65/15.5°C; solubility 0.10 mg/L at 24°C.

Rodger's Island in

Composition:

monochlorobiphenyls	3%
dichlorobiphenyls	13%
trichlorobiphenyls	28%
tetrachlorobiphenyls	30%
pentachlorobiphenyls	22%
hexachlorobiphenyls	4%

(1434)

composition of the water soluble fraction (WSF)			%	
monochloro isomers	137 µg/L	or	19	
dichloro isomers	224 µg/L	or	32	
trichloro isomers	220 µg/L	or	31	
tetrachloro isomers	116 µg/L	or	17	
pentachloro isomers	6 µg/L	or	1	
total WSF	702.7 µg/L		100	(1909)

:1 wt % of chlorine.

C. WATER POLLUTION FACTORS:

Control methods: calculated half-life based on evaporative loss for a water depth of 1 m at 25°C: 12 h. (330)

Aquatic reactions: partition coefficient to natural sediments.

sediment	*organic carbon %*	*partition coefficient*	
Oconee River	0.4	540	
USDA Pond	0.8	1,210	
Doc Run Pond	1.4	1,090	
Hickory Hill Pond	2.4	1,250	(1068)

(1909)

D. BIOLOGICAL EFFECTS:

Bioaccumulation: fathead minnows (from water) 8 m BCF 32,000–274,000. (1838)

Toxicity:

(997)

CRUSTACEANS:

amphipod *(Gammarus fasciatus)*	4d LC_{50},F	0.010 mg/L

crayfish *(Orconectes nais)*	7d LC_{50},S	0.030 mg/L
INSECTS:		
naiad of damselfly *(Ischnura fasciatus)*	4d LC_{50},F	0.40 mg/L
naiad of dragonfly (*Macromia* sp.)	7d LC_{50},S	0.80 mg/L

FISHES:

LC_{50},F mg/L d →	*5*	*10*	*15*	*20*	*25*	*30*	
rainbow trout	0.067	0.048	0.018	0.010	0.012		
bluegills			0.164	0.125	1.120	0.084	
channel catfish			0.219	0.150	0.132	0.087	(1617)

harlequin fish *(Rasbora heteromorpha)*

mg/L	*24 h*	*48 h*	*96 h*	
LC_{10},F	0.63	0.275	–	
LC_{50},F	0.96	0.6	0.37	(331)

cutthroat trout: 96h LC_{50},S 5.4 mg/L.

rainbow trout: acute oral toxicity >1.5 g/kg. (1617)

aroclor 1248

CAS 12672-29-6

Composition:

dichlorobiphenyls	2%	
trichlorobiphenyls	18%	
tetrachlorobiphenyls	40%	
pentachlorobiphenyls	36%	
hexachlorobiphenyls	4%	(1837)

C. WATER POLLUTION FACTORS:

Control methods: calculated half-life based on evaporative loss for a water depth of 1 m at 25°C: 9.5 h. (330)

Complete dechlorination of aroclor 1248 was obtained with 69% nickel on Kieselguhr in the presence of sodium hydroxide and 50 atm of hydrogen at 115°C for 6 h.

D. BIOLOGICAL EFFECTS:

Bioaccumulation:

Pimephales promelas 8m BCF 60,000–120,000 (1919, 1838)

channel catfish:

exposure (d)	*BCF (conc. in water 0.0058 µg/L)*	
7	3,500	
14	8,000	
28	29,000	
56	34,000	
77	56,370	(1617)

Toxicity:

CRUSTACEANS:

amphipod *(Gammarus fasciatus)* 4d LC_{50} 0.052 mg/L (1617)

FISHES:

	exposure (d)	*LC_{50} mg/L*
rainbow trout	5	0.054
	10	0.038
	15	0.016
	20	0.0064
	25	0.0034
bluegills	5	0.136
	10	0.115
	15	0.111
	20	0.106

	25	0.100	
	30	0.078	
fathead minnow larvae *(Pimephales promelas)*	30d	4.7 µg/L	(1919)
channel catfish	10	0.121	
	15	0.121	
	20	0.115	
	25	0.104	
	30	0.075	
Cutthroat trout	96h	5.7 mg/L	(1617)

Rainbow trout: acute oral toxicity: (1617)
>1.5 g/kg

aroclor 1254

CAS 27323-18-8

A. PROPERTIES: solubility 0.057 mg/L at 24°C.

Composition:

tetrachlorobiphenyls	11%	
pentachlorobiphenyls	49%	
hexachlorobiphenyls	34%	
heptachlorobiphenyls	6%	(1837)

composition of the water soluble fraction (WSF)		%	
trichloro isomers	1.8 µg/L	or 2.6	
tetrachloro isomers	28 µg/L	or 40	
penta- and hexachloro isomers	40 µg/L	or 57	
total WSF	69.8 µg/L	100	(1909)

C. WATER POLLUTION FACTORS:

Control methods: calculated half-life based on evaporative loss for a water depth of 1 m at 25°C: 10 h. (330)

Dechlorination was achieved in 2-propanol with 2.0 mmol $NiCl_2$, 60 mmol $NaBH_4$, and 0.3 mmol aroclor 1254. (1551)
Biphenyl constituted 97% of the reaction products, and monochloro- and dichlorobiphenyls the remaining products.

Biodegradation: biodegradation at 0.05 mg/L:

	normal sewage	adapted sewage	
after 24 h	0%	52%	
after 135 h	0%	43%	(997)

Impact on biodegradation processes: Effect on the degradation of glucose by a mixed culture derived from A.S.:

conc., mg/L	*increase in lag period*	*respiration rate*	
1	0 hours	100%	
10	0 hours	110%	
100	0 hours	135%	
1,000	>200 hours	0%	(997)

D. BIOLOGICAL EFFECTS:

Bioaccumulation: BCF for aquatic invertebrates:

		exposure period d				
species	*conc. in water, µg/L*	*1*	*4*	*7*	*14*	*21*
daphnid	1.1	2,100	3,800	–	–	–
amphipod	1.6	4,400	5,200	6,000	6,300	6,200
crayfish	1.2	160	240	350	500	750
grass shrimp	1.3	1,300	1,900	2,000	2,200	2,600
stonefly	2.8	640	710	740	750	740
dobsonfly	1.1	300	1,000	1,260	1,460	1,500
mosquito	1.5	2,300	3,400	3,500	–	–
phantom midge	1.3	2,400	2,500	2,600	2,700	–

BCF	
6,500	
12,000	
28,000	
42,500	
61,190	(1617)
00–47,000	(1531)
0–238,000	(1436)
0–307,000	(1838)
00–46,000	(1437)
10 ppb	(2350)
0.20 mg/L	
1.0 mg/L	(1617)
0.94 ppb	
3.5 ppb	
5 ppb	
5 ppb	
2.4 mg/L	
0.10 mg/L	
.003 mg/L	
30 µg/L	(1573)
$_{50}$,F mg/L	
6.2 µg/L	(1531)
0.160	
0.064	
0.039	
0.027	
0.303	
0.260	
0.239	
0.177	
0.303	
0.286	
0.293	
0.181	
0.139	
; 6.2 mg/L	
1.45 mg/L	
; 1.1 mg/L	(331)
42 mg/L	(1617)
>1.5 g/kg	
10 mg/L	
3.2 mg/L	(1861)
–1.28	
–1.95	
–1.77	(2644)

aroclor 1260

CAS 11096-82-5

A. PROPERTIES: solubility 0.080 mg/L at 24°C.

Composition:

pentachlorobiphenyls	12%	
hexachlorobiphenyls	38%	
heptachlorobiphenyls	41%	
octachlorobiphenyls	8%	
nonachlorobiphenyls	1%	(1837

C. WATER POLLUTION FACTORS:

Control methods: calculated half-life based on evaporative loss for a water depth of 1 m at 25°C: 10 h. (330

D. BIOLOGICAL EFFECTS:

FISHES:

fathead minnow larvae	30d LC_{50},F:	3.3 µg/L	
	250d BCF:	270,000	(1530
rainbow trout	30d LC_{50},F:	51 µg/L	
bluegill	30d LC_{50},F:	400 µg/L	
channel catfish	30d LC_{50},F:	433 µg/L	
cutthroat trout	96h LC_{50},S:	61 mg/L	(1617
rainbow trout: acute oral toxicity:		>1.5 g/kg	

aroclor 1262

CAS 37324-23-5

A. PROPERTIES: solubility 0.052 mg/L at 24°C. (166

D. BIOLOGICAL EFFECTS: Harlequin fish: 96h LC_{10},F not toxic below 100 mg/L. (33

arquad (quaternary ammonium salts; trimethylstearylammoniumchloride; trimethyloctadecylammoniumchloride)

$C_{21}H_{46}N{\bullet}C1$

CAS 112-03-8

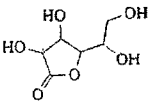
USES: trademark for a series of quaternary ammonium salts containing one or two alkyl groups ranging from C_8 to C_{18}; cor rosion inhibitors; emulsifiers; germicides and sanitizing agents; textile fabric softeners.

A. PROPERTIES: molecular weight 348.13.

C. WATER POLLUTION FACTORS:

Biodegradation: at ±18 mg/L, no degradation after 28 d exposure to nonadapted sewage. (488)

ascorbic acid (vitamin C)



$C_6H_8O_6$

CAS 50-81-7

232 atrazine

$C_9H_{17}N_5O$

CAS 1610-17-9

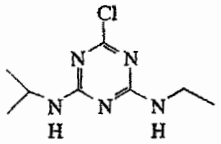
USE: selective herbicide used to protect sugarcane.

A. PROPERTIES: molecular weight 211.27; melting point 94–96°C; solubility 1,800 mg/L at 20°C; P_{oct} 1.98; 2.69.

C. WATER AND SOIL POLLUTION FACTORS: in groundwater wells in the U.S.A.—150 investigations up to 1988:

median of the conc.'s of positive detections for all studies	0.1 μg/L	
maximum conc.	0.1 μg/L	(2944)

atrazine (2-chloro-4-ethylamino-6-isopropylamino-*s*-triazine)



$C_8H_{14}ClN_5$

CAS 1912-24-9

USES: Most widely used chemical for pre-emergence weed control in corn. In Hawaii, it is important to the culture of sugar cane, pineapple, and macadamia nut.

A. PROPERTIES: colorless crystals; molecular weight 215.7; melting point 173–175°C, vapor pressure 3×10^{-7} mm at 20°C; 4×10^{-7} hPa at 20°C; solubility 33– 35 mg/L; 70 ppm at 25°C, d 1,2 kg/L at 20°C; log P_{oct}: 2.64; 2.23; 2.35; 2.4; 2.61; 2.63; 2.68.

B. AIR POLLUTION FACTORS:

Cuticle-water distribution coefficient (log K_{cw}) for the cuticular membrane of *Citrus aurantium:* log K_{cw}: 2.19. (2448)
Cuticle-air distribution coefficient (log K_{cw}) for the cuticular membrane of *Brassica Oleracea L:* log K_{ca}: 9.13.00
Leaf-air distribution coefficient (log K_{la}) for the whole leaf of *Brassica oleracea* L.: log K_{la}: 7.28.

C. WATER AND SOIL POLLUTION FACTORS:

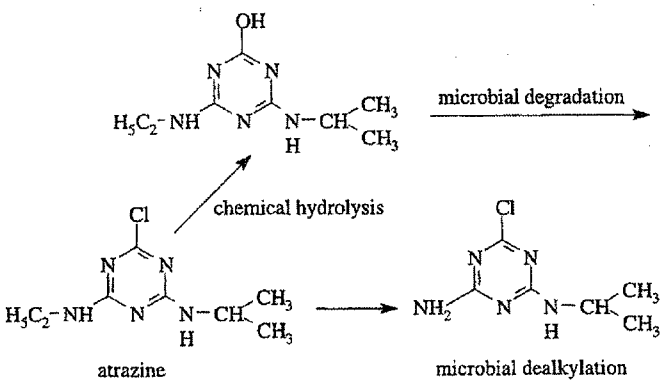
Mobility: *Soil sorption:* K_{oc}: 45– 63; 100 (7045; 2576)

In rivers in UK (1986): 139 samples from 70 river sites yielded 83 positive values (detection limit: 0.025 μg/L): median of positive values: 0.11 μg/L; maximum: 1.12 μg/L (2711)
Reductive dehalogenation in anaerobic lake sediment suspension at 20°C in the dark: half-life: 4.2 d (2700)
In groundwater wells in the USA—150 investigations up to 1988:

median concn of positive detections for all studies	0.5 μg/L	
maximum concn	40 μg/L	(2944)

- Microorganisms in aerobic incubations of alluvial aquifer sediment mineralized: 9–14% of added glucose in 24 h compared with <0.1–1.5% of added atrazine (ethyl ^{14}C labeled) and <0.1% of added atrazine (U-ring ^{14}C labeled) (2572)

Biodegradation and aqueous reactions: in submerged soils: in 90 d 0.005% of atrazine-^{14}C was recovered as $^{14}CO_2$ (from ring labeled atrizine); 48– 85% of atrazine was hydrolyzed in 30 d, depending on soil type. Chemical hydrolysis of atrazine to hydroxyatrazine is the principal pathway of detoxication in soil. Biological dealkylation without dehalogenation occurs simultaneously, leading to 2-chloro-4-amino-6-isopropylamino-*s*-triazine:

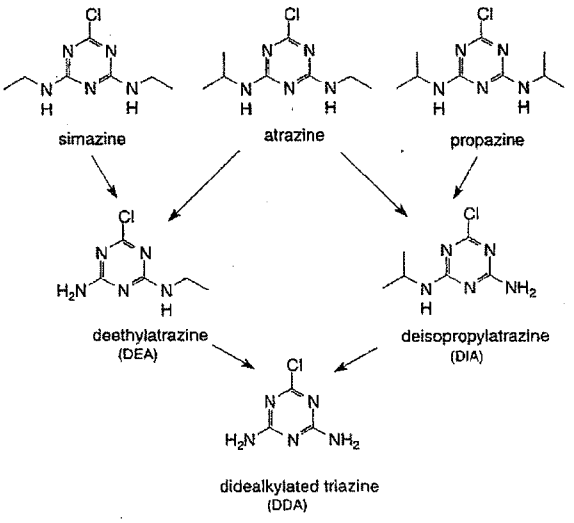


(1307)

Biodegradation in soil			
in greenhouse at 23–26°C at constant light at initial conc. of 5–10 mg/kg soil, experiment time 50 d:	$t_{1/2}$ d		
in sandy soil	30		
in organic-rich orchard soil	40		
in agricultural soil	41		
in soil from volcanic area	20		
in field experiments	60 (dissipation $t_{1/2}$)		(7045)
Dissipation periods in sandy soil in the field	DT_{50} (d)	DT_{90} (d)	
	19–26	133–193	(6020)

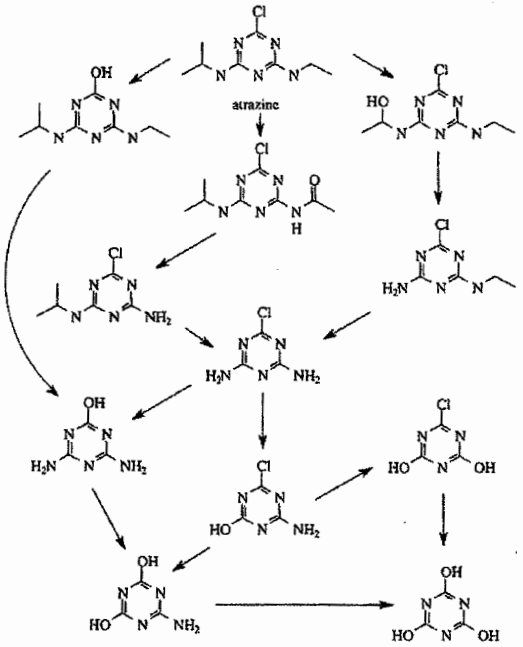
75–100% disappearance from soils: 10 months. (1815)

The preferential dealkylation pathway of the *s*-triazine herbicides in the unsaturated zone is the removal of an ethyl side chain relative to an isopropyl side chain. It is hypothesized that deethylation reactions may proceed at 2–3 times the rate of deisopropylation reactions.



Dealkylation reactions of atrazine, simazine, and propazine to deethylatrazine (DEA), deisopropylatrazine (DIA), and didealkylatrazine (DDA). (2952)

Phototransformation under simulated sunlight in the presence of soil extract (aqueous humic acid solution). The following degradation pathway is proposed (2914)



The presence of humic substances in aqueous solution at very low concentration (10 ppm of organic carbon) increases the photolytic degradation of atrazine 3 times under simulated solar light. The dehalogenation path accounts for most of the initial degradation process, but dealkylated and deaminated products have also been detected in significant amounts. (2914)

Water treatment:

Initial concentration, µg/L	Treatment method	% removal	
50–100	Chlorination	100	
0.0001	Chlorination	0	
not reported	river bank filtration	low	
not reported	Ozonization + flocculation	±10	
not reported	Flocculation	±5	
not reported	Activated carbon	100	
not reported	Aeration	not significant	(2915)

D. BIOLOGICAL EFFECTS:

BACTERIA:

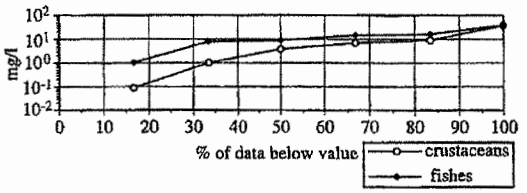
Nitrification inhibition in soil (1% organic carbon)	14 d IC_{52}	50 mg/kg	(7050)
Biotox test *Photobacterium phosphoreum*	5 min EC_{10}	7.5 mg/L	
Microtox test *Photobacterium phosphoreum*	5 min EC_{10}	13 mg/L	(7023)
Pseudomonas putida	16 h EC_0	>10 mg/L	(329)

ALGAE:

Chlamydomonas reinhardi	Lethal, 24–48 h	216 µg/L	
Selenastrum capricornutum:			
inhib. of oxygen evolution	EC_{50}	0.0697 mg/L; 0.854 mg/L	
growth inhib.	EC_{50}	0.0587 mg/L; 0.41 mg/L	
OECD 209 closed system	EC_{50}	>0.045 mg/L	(2624)
Selenastrum capricornutum	72 h EC_{50}	0.2-0.22 mg/L	
	72 h EC_{100}	1.0 mg/L	(7024)

Microcystis aeruginosa	8 d EC_0	0.003 mg/L	(329)
Chlorococcum sp.	10 d EC_{50}	100 ppb technical acid	
Dunaliella tertiolecta	10 d EC_{50}	300 ppb technical acid	
Isochrysis galbana	10 d EC_{50}	100 ppb technical acid	
Phaeodactylum tricornutum	10 d EC_0	100–200 ppb technical acid	

CRUSTACEANS:



atrazine crust + fish

Frequency distributions for 24– 96 h LC_{50} values for crustaceans and fishes (n = 6) based on data from this and other works (3999)

Daphnia magna	48 h IC_{50}	>39 mg/L	(2625)

Bioaccumulation:

BCF:	snails:	2–15	
	algae:	10–83	
	fish:	3–10	(1891, 1892, 1893)
Chlorella fusca BCF (wet wt): 52			(2659)

FISHES:

bluegill	2 yr LC_{50},F	5.4–8.4 mg/L	at 27°C	
	MATC:	0.09 mg/L	at 27°C	
fathead minnows	1 yr LC_{50},F	11–20 mg/L	at 25°C	
	MATC:	0.21 mg/L	at 25°C	
brook trout:	1.5 yr LC_{50},F	4.0–6.0 mg/L	at 9–16°C	
	MATC:	0.06 mg/L	at 916°C	(448)
Cyprinodon variegatus	96 h LC_{50}	16 mg/L		
	MATC, early life stage	2.5 mg/L		(2643)
Menidia beryllina	96 h LC_{50}	1 mg/L		
	MATC life cycle	0.12 mg/L		(2643)

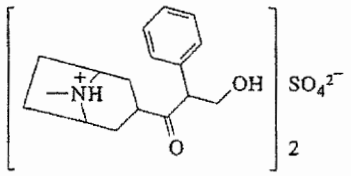
log BCF: fathead minnow: 0.90 (2606)

lowest NOEC per species	µg/L
Cyanophyta	1.5
Chlorophyta	15; 83
Branchiopoda	140
Malacostraca	60
Diptera	110
Pisces	65

(2906)

PLANTS: Bioconcentration factor for vegetation: log BCF_v: –2.00 (2644)

atropine sulfate monohydrate



(326)
(882)

BACTERIA:

Activated sludge respiration inhibition	EC_{50}	14 mg/L.	(2624)

(2787)

FISHES:

threespine stickleback	4h LC_{100}	2 mg/L	
steelhead trout	2h LC_{100}	2 mg/L	(9837)

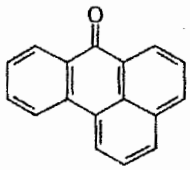
(32)

benzaminocetic acid *see* hippuric acid

(92)

benzanthrone

(93)



(192)

$C_{17}H_{10}O$

CAS 82-05-3

(1900)
(329)
(1900)

USE: dyes.

A. PROPERTIES: pale yellow needles; melting point 170°C; molecular weight 230.27.

(1900)
(901)

B. AIR POLLUTION FACTORS:

Ambient air quality: glc at Botrange (Belgium): woodland at 20–30 km from industrial area—June 1977: 0.18 ng/m^3. (1233)

(226)

1-benzazine *see* quinoline

(2709)

benzene

n chloride;

C_6H_6

CAS 71-43-2

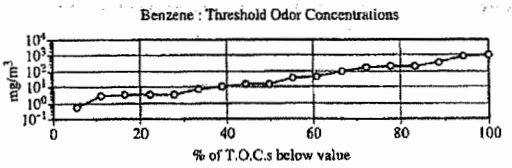
MANUFACTURING SOURCE: petroleum refinery; solvent recovery plant; coal tar distillation; coal processing; coal coking. (347)

USES AND FORMULATION: mfg. styrene, phenol, detergents, organic chemicals, pesticide, plastics and resins, synthetic rubber, aviation fuel, pharmaceuticals, dye, explosives, PCB gasoline, tanning, flavors and perfumes, paints and coatings; nylon intermediates; food processing; photographic chemicals. (347)

a general

A. PROPERTIES: colorless liquid; molecular weight 78.11; melting point 5.5°C; boiling point 80.1°C; vapor pressure 76 mm at 20°C, 60 mm at 15°C, 118 mm at 30°C; vapor density 2.77; d 0.88 at 20/4°C; solubility 1,780 mg/L at 20°C; saturation concentration in air 319 g/m^3 at 20°C, 485 g/m^3 at 30°C; log P_{oct} 2.13 at 20°C, 2.64; 2.73; log H –0.65 at 25°C.

B. AIR POLLUTION FACTORS: 1 mg/m^3= 0.31 ppm, 1 ppm= 3.26 mg/m^3.



(2, 3, 4, 5, 9, 278, 291, 307)

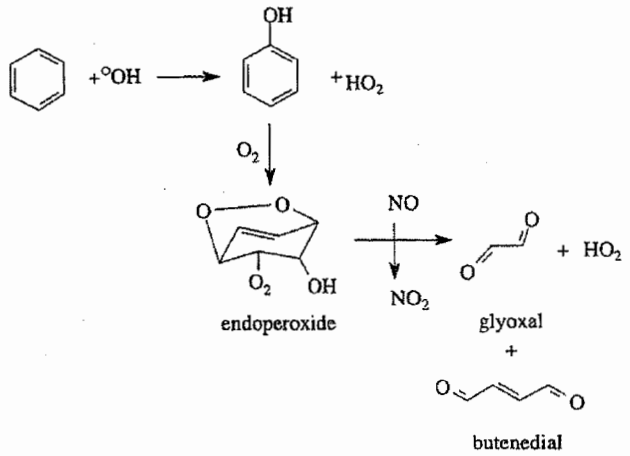
$PIT_{50\%}$: 2.14 ppm
$PIT_{100\%}$: 4.68 ppm (2)
distinct odor: 310 mg/m^3= 90 ppm (278)
human odor perception: 3.0 mg/m^3= 1 ppm
animal chronic exposure: adverse effect: 3.2 mg/m^3 (170)

Atmospheric reactions: R.C.R.: 0.276. (49)

reactivity: HC cons.: ranking: 0.5
NO ox.: ranking: 0.04–0.15 (63)

Atmospheric half-lives:
for reactions with OH°: 5.7 d
for reactions with O_3: 170,000 d (2716)

Atmospheric reactions: Only the reaction with hydroxyl radicals is important: rate constants (K_{OH}) between 1,300 and 2,350 have been reported with an average of 1,800 (ppm^{-1}, min^{-1}). Based on this latter value, an average lifetime of 5.3 d can be calculated for the Netherlands. The following reaction pathway is proposed:



(2701)
Natural sources: volcanic eruptions, vegetation, forest fires: a benzene concentration of 35 µg/m^3 was measured in the plume of a forest fire at a distance of 6 km of the seat of the fire. (2701)
glc's Pt Barrow, Alaska, Sept. 1967: not detectable to 0.4 ppb (101)

Manmade sources:
In cigarette smoke: 150-205 mg/m^3
in main stream: 0.01-0.1 mg/cigarette
in side stream: 0.05-0.49 mg/cigarette (2701)
500 µg/cigarette (2421)
In flue gases of a municipal waste incinerator plant: 15 µg/m^3 = 1.3% of total organic carbon emissions. (7048)

Atmospheric emissions in the Netherlands in 1981:
percentage

exhaust gases from car engines	85	
production, use, and transport of benzene and derivatives	10	
remaining traffic	2	
production and transport of petrol	1	
storage and handling at gasoline stations	1	
evaporation from car tanks	1	(2701)

diesel engine: 2.4% of emitted HCs (72)

rotary gasoline engine: 1.3% of emitted HCs
reciprocating gasoline engine: 2.2% of emitted HCs (78)
expected glc's in U.S. urban air: range: 10 to 50 ppb (102)
emitted by household central heating system on gasoil:
~20 ppm at 7% CO_2
6 g/kg gasoil at 6% CO_2
2.2 g/kg gasoil at 7% CO_2 (182)
in gasoline exhaust: 0.1 to 42.6 ppm (partly methylvinylketone) (195)
in gasoline: 1.8–5% (312, 34)
in exhaust of gasoline engines: 62-car survey: 2.4 vol% of total exhaust HCs (391)
exhaust emissions from 1975 GM models equipped with bead-type converters:

% of total hydrocarbons:	avg 2.7%,	range 1–7% (1975 federal test procedure)
mg/mile:	avg 20,	range 8–75

exhaust emission from noncatalyst cars (mostly 1974 GM models)

of total hydrocarbons:	4.6% avg	
mg/mile:	113 avg	(1386)

According to an EPA source inventory published in 1989, 85% of benzene emissions in the U.S.A. are from mobile sources, of which 70% are from exhaust, 14% from evaporative emissions, and 1% from vehicle refueling. Benzene averaged 3–4% of total hydrocarbons. (2417)

automotive emissions:
precatalyst cars: 114–153 mg/mile
catalyst cars: 5–32 mg/mile
1983–87 in-use vehicles: 4.8–15 mg/mile
1983–87 in-use trucks: 9.5–14 mg/mile (2416)

average emission by model year:

model year	emission, mg/mile
1981/1982	27
1983/1984	13
1985	8.6
1986	9.6
1987	6.6

(2416)

In 4 municipal landfill gases in Southern Finland (1989–90 data): avg 0.17–9, max 11 mg/m^3. (2605)

Ambient air quality:
glc's in Netherlands:
in tunnel Amsterdam—1973: avg 6 ppb ($n = 3$)

in tunnel Rotterdam—1974.10.2:	avg	25 ppb ($n = 12$)
	max	33 ppb
The Hague—1974.10.11:	avg	13 ppb ($n = 12$)
	max	29 ppb
Roelofarendsveen—1974.9.11:	avg	2 ppb ($n = 12$)
	max	3 ppb

(1231)

glc's in the U.S.A. during winter 1977–78:

	averages	*range (8 h average)*
urban/suburban areas:	<0.5–3.6 ppb	<0.5–12.1 ppb
rural areas:	<0.5–0.6 ppb	<0.5–1.8 ppb
remote areas:	<0.5–0.7 ppb	<0.5–2.0 ppb

(1401)

glc's in Los Angeles 1966:

avg:	0.015 ppm (n = 136)	
highest value:	0.057 ppm	(1319)

Indoor/outdoor glc's winter 1981/1982 and 1982/1983 the Netherlands:

$\mu g/m^3$	*median*	*maximum*	
pre-war homes	7	24	
post-war homes	7	148	
<6-year-old homes	5	53	
outdoors	3	7	(2668)

Indoors/outdoors Germany 1980: n = 15, averages of 1 to several d

$\mu g/m^3$	*mean*	*range*	
in the kitchen	15	6–27	
in the other rooms	18	6–14	
outdoors	29	4–33	(2669)

Inside and outside 15 living rooms in Northern Italy (1983–84):

4–7 d averages	*lowest*	*mean*	*highest value, $\mu g/m^3$*	
indoor	5	52	204	
outdoor	3	20	67	(2756)

Photochemical reaction: estimated lifetime under photochemical smog conditions in SE England: 28 h. (1699, 1707)

Control methods:
platinized ceramic honeycomb catalyst: ignition temp.: 180°C
inlet temp. for 90% conversion: 250–300°C (91)

Incinerability:

Temperature for 99% destruction at 2.0 sec residence time under oxygen-starved reaction conditions: 1,150°C

Thermal stability ranking of hazardous organic compounds: rank 3 on a scale of 1 (highest stability) to 320 (lowest stability) (2390)

Partition coefficients:

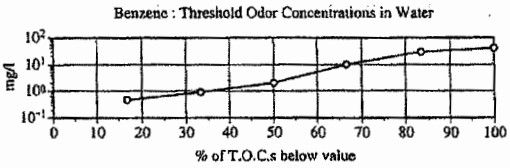
$K_{air/water}$	0.25	
Cuticular matrix/air partition coefficient*	430 ± 0	(7077)

* experimental value at 25°C studied in the cuticular membranes from mature tomato fruits (*Lycopersicon esculentum* Mill. cultivar Vendor)

C. WATER POLLUTION FACTORS:

BOD_5:	0; 0; 10; 24; 70% ThOD	(23, 41, 27, 220, 274, 277)
	58% ThOD. (acclim.)	(23)
BOD_{10}:	67% bio.-ox. (acclim.)	(23)
	27; 39% ThOD. (nonacclim.)	(23, 256)
BOD_{15}:	76% ThOD. (acclim.)	(23)
	24% ThOD. (nonacclim.)	(23)
BOD_{20}:	80% ThOD. (acclim.)	(23)
	29% ThOD. (nonacclim.)	(23)
$BOD_{35}^{25°C}$:	61% ThOD	(62)
$BOD_{35}^{25°C}$:	51% ThOD in seawater/inoculum: enrichment cultures of hydrocarbon oxidizing bacteria	(521)
COD:	8; 45% ThOD	(27, 23)
	19% ThOD	(220)
	69% ThOD ASTM procedure	(272)
	93% ThOD	(272)
	33% ThOD (0.05 n $K_2Cr_2O_7$)	(274)
TOC:	40% ThOD	(220)
ThOD:	3.10	(23)

(1319)



(2668)

Biodegradation: CO_2 in estuarine water: in June after 24 h incubation.

Concentration (µg/L)	*Degradation rate, (µg/L/d) ×10³*	*Turnover time, d*	
6	200±10	30	
12	260±25	46	
24	330±30	75	(381)

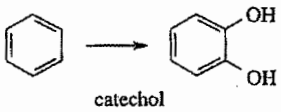
(2669)

Incubation with natural flora in the groundwater in presence of the other components of high-octane gasoline (100 µl/L).

(2756)

Biotic transformation in water: the following pathways are suggested: hydroxylation of the hydrocarbon ring:

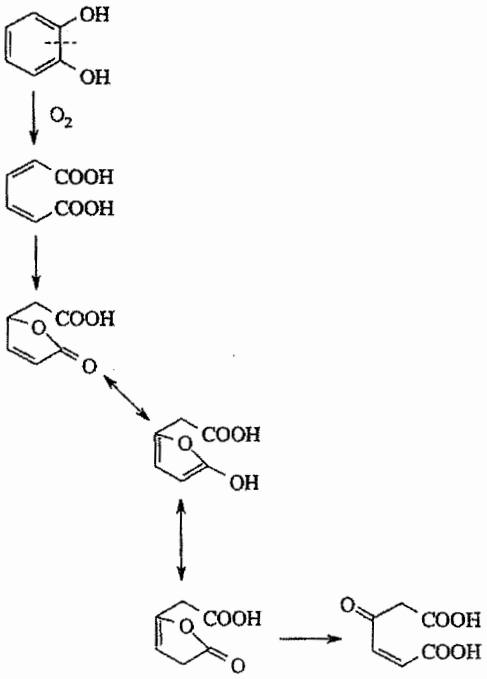
(1699, 1707)



(91)

ortho-fission of catechol:

150°C



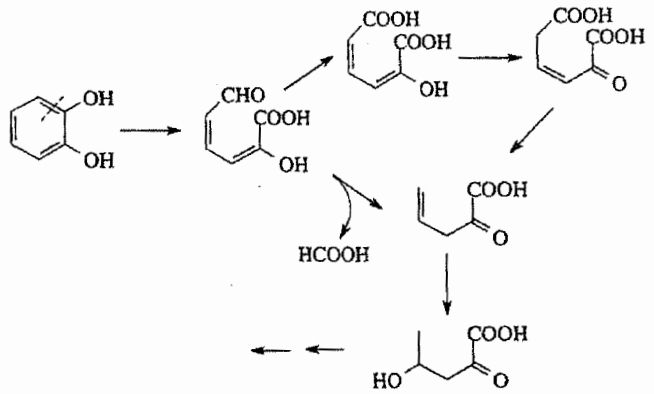
120 (lowest stability)
(2390)

(7077)
Mill. cultivar Vendor)

(23, 41, 27, 220, 274, 277)
(23)
(23)
(23, 256)
(23)
(23)
(23)
(23)
(62)

(521)
(27, 23)
(220)
(272)
(272)
(274)
(220)
(23)

meta-fission of catechol:



(2701)

Photolysis in water: immediately below the water level, the calculated half-life is ± 80 d based on reaction with the OH radical; the half-life increases linearly with depth as a result of decreasing light intensity. (2701)

In estuaries at conc. of 6–24 µg/L, half-life: 15–38 d

In mesocosms at 5.5 m depth in the sea at 0.2–4 µg/L, half-lives:

at 3–7°C	13 d
at 8–16°C	23 d
at 20–22°C	3.1 d

At larger depths the half-lives increased proportionately. (2701)

Water treatment:

Ozonation: surface water containing 80 µg/L treated with 2.8 mg ozone/L resulted in 97% removal (2701)

Activated sludge treatment: 99% removal (2701)

Reverse osmosis: 76–87% rejection was obtained by a low-pressure thin-film compos- ite polyamide membrane FT-30 in spiral wound configuration at influents of 10–25 mg/L at ambient temp (2630)

initial concentration, µg/L	*treatment method*	*% removal*	
371–750	river bank filtration	80–82	
120–416	activated carbon	17–95	(2915)

Aerobic degradation of mixed organic wastes by a propane-fed bioreactor: >90% within 21 d at 22°C and initial conc. of 0.086 mg/L. (2432)

Micelle-water partition coefficient (K_{mw}) for the anionic surfactant dodecylsulfate: log K_{mw}: 2.88–3.06 (on mass basis), 2.11 (on vol basis). (2361)

Disappearance in soil at 100 mg/kg and 20°C under aerobic laboratory conditions:

Half-life: >2 d (2366)

Degradation half-lives:	3.1–23 d in marine mesocosm	(2367)
	8.6 d in activated sludge	(2368)

Waste treatment: Aerobic slurry bioremediation reactor with mixed aeration chamber, treating a petrochemical waste sludge at 3.5 to 7.5% solids containing approx. 25% oil and grease and 0.5 to 2.5 g of waste material per gram of microorganisms, at 22–24°C during batch treatment:

mixed liquor: infl.: 13 mg/L; effl. after 15 d: <1 mg/L

waste residu: infl.: 290 mg/kg; effl. after 90 d: <1 mg/kg

vapor phase: infl.: 83–156 ppm; after 4 d: 5–10 ppm; after 9 d: nd-0.3 ppm (2800)

Water quality:

in river Maas at Eysden (Netherlands) in 1976:	median: 0.1 µg/L; range: n.d. to 5.7 µg/L	
Keizersveer (Netherlands) in 1976:	median: 0.1 µg/L; range: n.d. to 1 µg/L	(1368)

in Lake Zürich (Switzerland): at surface: 28 ppt; at 30 m: 22 ppt

in Zürich area: spring water: 18 ppt; ground water: 45 ppt; tap water: 36 ppt (513)

Aquatic reactions: evaporation: Calculated half-life in water at 25°C and 1 m depth, based on evaporation rate of 0.144 m/h: 4.81 h; based on evaporation rate of 0.137 m/h: 5.03 h. (437)

Soil adsorption: Freundlich constants for benzene sorption after 16 h incubation at concentrations 10–1,000 ppb:

adsorbent	*K*	*1/n*	
Hastings silty clay loam	2.4	0.89	
Overton silty clay loam	1.8	0.94	
Al-saturated montmorillonite	31	1.8	
Ca-saturated montmorillonite	4.4	0.99	(1862)

Waste water treatment:

A.S.: 33% ThOD of 500 ppm by phenol acclimated A.S. after 12 h aeration (26)

A.C.: adsorbability: 0.08 g/g, 95% reduction, infl.: 416 mg/L, effl.: 21 mg/L (32)

anaerobic lagoon: 13 lb/d/1,000 cu ft: infl.: 10 mg/L, effl.: 5 mg/L (37)

ion exchange: adsorption on Amberlite X AD-2: retention efficiency: 100% at 100 ppm influent conc. (40)

air stripping constant: K= 1.71 d^{-1} at 100 mg/L (82)

A.S., Sd. BOD, 14 d acclim.: 2% of ThOD after 5 d at 20°C

A.S., W, 14 d acclimation: 3% of ThOD after 1/4 d at 20°C, feed: 50–200 mg/L (93)

air flotation after chemical addition: 78% removal (173)

A.C.: influent, ppm	*carbon dosage*	*effluent, ppm*	*% reduction*	
500	10×	27	95	
250	10×	23	91	
50	10×	20	60	(192)

Manmade sources:

Göteborg (Sweden) sew. works 1989–1991: infl.: 0.1–5 μg/L; effl.: <0.5 μg/L (2787)

Landfill leachate from lined disposal area (Florida 1987–'90): mean conc. 0.10; 1.9 μg/L (2788)

In digested sewage sludge: U.K. 1993: n = 12

mean:	0.084 mg/kg dry wt	SD:	0.116 mg/kg dry wt	
	2.87 μg/L wet volume	SD:	3.97 μg/L wet volume	(2946)

In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 sludges ranged from 0.024 to 0.48 mg/kgdw.; mean: 0.058 mg/kg dw mean value of sludge compost: 0.0046 mg/kg dw. (7000)

Degradation in soil: biodegradation in methanogenic aquifer at 17°C and initial conc. of 613 μg/L: $t_{1/2}$ = 27 weeks. (2614)

Fate of ^{14}C-labeled compound in a laboratory soil-plant system (7 d):

volatilization:	0.25%
mineralization:	62.2%
soluble metabolites in soil:	0.93%
bound residues:	9.99%
uptake by barley:	0.065%
uptake by cress:	0.24% (2616)

Biodegradation half-lives in nonadapted aerobic subsoil:

groundwater Florida:	12 d	
river Oklahoma:	24 d	
sand Texas:	>161 d	
sand Ontario:	48 d	(2695)

Impact on biodegradation processes:

Effect on the mineralization of acetate in anaerobic river sediment at 20°C:

toxic effects:	EC_{50}: 3,500 mg/kg dry sediment	
	EC_{10}: 1,200 mg/kg dry sediment	
inhibition of mineralization:	IC_{50}: 1,700 mg/kg dry sediment	
	IC_{10}: 480 mg/kg dry sediment	(2693)

Inhibition of acetoclastic methanogenesis in a granular sludge:
IC_{50}: 1,500 mg/L (2694)

Toxic effect of benzene on the mineralization of the following chemicals in methanogenic river sediment:

chemical	*EC_{50}*	
4-chlorophenol	2,500 mg/kg dw	
benzoate	590 mg/kg dw	
acetate	3,500 mg/kg dw	
chloroform	2,600 mg/kg dw	
methanogenesis	>10,000 mg/kg dw	(2961)

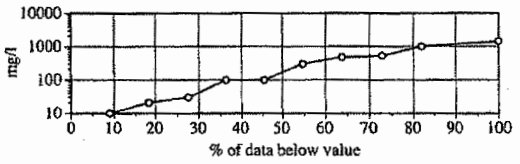
Soil sorption: K_{oc}: 38–53 at 1.0 mg/L (2588)

D. BIOLOGICAL EFFECTS:

BACTERIA:

Pseudomonas putida	16h EC_0	92 mg/L	(1900)
Biotox™ test *Photobacterium phosphoreum*	5 min EC_{50}	2,600 mg/L	
Microtox™ test *Photobacterium phosphoreum*	5 min EC_{50}	531 mg/L	(7023)

ALGAE:



Frequency distribution of short-term EC_{50}/LC_{50} values for algae (n = 11) based on data presented in this and in other works (3999)

Microcystis aeruginosa	8d EC_0	>1,400 mg/L	(329)
Scenedesmus quadricauda	7d EC_0	>1,400 mg/L	(1900)

Chlorella vulgaris: 50% reduction of cell numbers vs controls, after 1-d incubation at 20°C: at 525 ppm
Inhibition of photosynthesis of a freshwater, nonaxenic unialgal culture of Selanastrum capricornutum
at 10 mg/L: 95% ^{14}C fixation (vs controls)
at 100 mg/L: 84% ^{14}C fixation (vs controls)
at 1,000 mg/L: 5% ^{14}C fixation (vs controls) (1690)

Tetrahymena pyriformis	24 h LC_{100}	1,000 mg/L	(1662)
Chlorella fusca	BCF	30 (wet wt)	(2659)

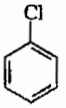
PROTOZOA:

Entosiphon sulcatum	72 h EC_0	>700 mg/L	(1900)
Uronema parduczi Chatton-Lwoff	EC_0	486 mg/L	(1901)

CRUSTACEAN:

BACTERIA: *Pseudomonas fluorescens*	24h EC_0	500 mg/L	(5649)
FISHES: rainbow trout (*Salmo gairdneri*)	12h LC_{50}	5.2 mg/L	
	24h LC_{50}	3.6 mg/L	
	48h LC_{50}	2.8 mg/L	
	96h LC_{50}	2.5 mg/L	(1913)
Leuciscus idus	48h LC_0	20 mg/L	
	48h LC_{100}	50 mg/L	(5649)
Gambusia affinis	24h LC_{50},S	8.9 mg/L	(5650)

chlorobenzene (phenylchloride)



C_6H_6Cl

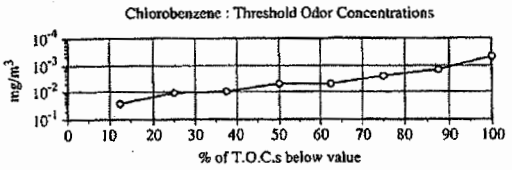
CAS 108-90-7

USERS AND FORMULATIONS: solvent recovery plants; intermediate in dyestuffs mfg.; mfg. aniline, insecticide, phenol, chloronitrobenzene. (347)

A. PROPERTIES: colorless liquid; molecular weight 112.56; melting point -45 °C; boiling point 132 °C; vapor pressure 8.8 mm at 20 °C, 11.8 mm at 25 °C, 15 mm at 30 °C, 12 hPa at 20 °C, 20 hPa at 30 °C, 53 hPa at 50 °C; vapor density 3.88; d 1.11 at 20/4°C; solubility 500 mg/L at 20°C, 488 mg/L at 30°C; saturation concentration in air 54 g/m^3 at 20°C, 89 g/m^3 at 30°C; log P_{oct} 2.84 at 20°C; log H -0.74 at 25°C.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.217 ppm, 1 ppm = 4.678 mg/m^3.

Odor: characteristic: quality: chlorinated mothballs, aromatic.



(57, 73, 279, 298, 307, 610, 748, 815, 838)

human odor perception:	0.4 mg/m^3 = 0.09 ppm	
human reflex response:	no response: 0.1 mg/m^3	
	adverse response: 0.2 mg/m^3	
animal chronic exposure:	no effect: 0.1 mg/m^3	
	adverse effect: 1.0 mg/m^3	(170)
O.I. at 20°C: 52,600		(316)

Incinerability:

Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 990°C.

Thermal stability ranking of hazardous organic compounds: rank 19 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

Manmade sources: in 4 municipal landfill gases in Southern Finland (1989–1990 data): avg 0.01–0.19, max. 0.33 mg/m^3. (2605)

Ambient air quality:
Indoor/outdoor glc's winter 1981–1982 and 1982–1983, the Netherlands:

	median	*maximum (all in µg/m³)*	
pre-war homes	<0.4	3	
post-war homes	<0.4	<0.4	
homes <6 years old	<0.4	27	
outdoors	<0.4	<0.4	(2668)

Partition coefficients

$K_{air/water}$	0.15	
Cuticular matrix/air partition coefficient*	3300 ±0	(7077)

* experimental value at 25 °C studied in the cuticular membranes from mature tomato fruits (*Lycopersicon esculentum* Mill. cultivar Vendor)

C. WATER POLLUTION FACTORS:

BOD_5:	1.5% ThOD std. dil. sew.	(41, 27, 298)
COD:	20% ThOD.	(27)
ThOD:	2.06.	(27)
Impact on biodegradation processes:	at 100 mg/L, no inhibition on NH_3 oxidation by *Nitrosomonas* sp.	(390)
Reduction of amenities:	T.O.C.: 0.1 mg/L.	(296, 903)

Water quality:
in Zürich Lake: at surface: 3 ppt; at 30 m depth: 12 ppt
in Zürich area: in groundwater: 14 ppt; in tap water: 6 ppt (513)

in Delaware River (U.S.A.): conc. range:	winter:	7.0 ppb	
	summer:	n.d.	(1051)

in river Mass at Eysden (Netherlands) 1976: median: n.d.: range: n.d.–1.9 µg/L
in river Maas at Keizersveer (Netherlands) 1976: median: n.d.: range: n.d.–9.6 µg/L (1368)
in rivers in U.K. (1986): 139 samples from 70 river sites yielded 24 positive values (detection limit: 0.1 µg/L): median of positive values: 0.23 µg/L; maximum: 7.6µg/L (2711)

in Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 1.5 mg/kg of organic carbon
suspended sediments: 0.22 mg/kg of organic carbon
water: 18 ng/L (2646)

Manmade sources:
Occurrence in sewage sludges, NW England 1989:

urban	mean	57,300 µg/kg dry wt	
	SD	104,000 µg/kg dry wt	
urban/industrial	mean	7,010 µg/kg dry wt	(2953)

In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 sludges ranged from 0.003 to 0.20 mg/kg dw.; mean: 0.062 mg/kg dw mean value of sludge compost: ND. (7000)

Waste water treatment:
air stripping constant: $K = 0.969\ d^{-1}$ at 100 mg/L (82)

ring disruption by *Pseudomonas* at 200 mg/L:

parent:	100% in 58 h	
mutant:	100% in 14 h	(152)

Aerobic slurry bioremediation reactor with mixed aeration chamber, treating a petrochemical waste sludge at 3.5 to 7.5% solids containing approx. 25% oil and grease and 0.5 to 2.5 grams of waste material per gram of microorganisms, at 22–24°C during batch treatment: waste residue: infl.: 4.4 mg/kg; effl. after 90 d: <1 mg/kg. (2800)

Dimensionless distribution coefficient at initial conc. = 1 mg/L:

on mixed liquor:	290	
on primary waste water sludge:	480	
on anaerobically digested sludge:	290	(2395)

Degradation in soil and in sediment:

Disappearance in soil at 100 mg/kg and 20 °C under aerobic laboratory conditions: half-life: 2.1 d; confidence limits: 1.7-3.0 d (2366)

Reductive dechlorination in sediment under sulfate reducing conditions at 25 °C to benzene: half life period assuming peudo first order kinetics: 46 d. (7041)

Degradation half-lives: 75 d in sediment (2369)
4.6-21 d in marine mesocosm (2367)
7.9 d in activated sludge (2368)

Biodegradation half-lives in nonadapted aerobic subsoil:
sand Oklahoma: >539 d
coarse sand Oklahoma: 81; 242 d (2695)

Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
domestic sewage	Closed Bottle Test		20 d	50-60% ThOD	(9147)
A.S. industrial non adapted	Respirometric Test		5 d	30% ThOD	
			10 d	70% ThOD	
			15 d	>90% ThOD	(9149)
A.S.	Modified MITI Test		28 d	15% ThOD	(9146)
different sludges	Modified MITI Test	100 mg/L	28 d	0% ThOD	(9148)

Partition coefficients

Cuticular matrix/water partition coefficient**	500	(7077)
log K_{oc}	2.60	(2597)

** calculated from the Cuticular matrix/water partition coefficient and the air/water distribution coefficient

D. BIOLOGICAL EFFECTS:

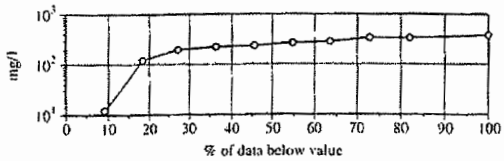
Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Fishes: *Cyprinus carpio*	150	8 weeks	4.3-40	whole body	
	15	8 weeks	3.9-23	whole body	(9148)
fathead minnow			447		(2606)

BACTERIA:

Pseudomonas putida	16h EC_0	17 mg/L	(1900)
A.S. respiration inhibition	30 min EC_{50}	140 mg/L	(2624)
A.S. oxygen consumption test	30 min EC_{50}	2,950 mg/L	(9146)
A.S. domestic ETAD Test	24d EC_{50}	17 mg/L	(9147)
Photobacterium phosphoreum	5 min IC_{50}	9.4 mg/L	(9153)
	10 in IC_{50}	20 mg/L	(9147)
	30 min IC_{50}	11 mg/L	(9147)
Aerobic heterotrophs	15h IC_{50}	310 mg/L	(9153)
Methanogens	48h IC_{50}	270 mg/L	(9153)
Nitrosomonas inhibition of N oxidation	24h IC_{50}	0.71 mg/L	(9153)

ALGAE:

Scenedesmus subspicatus	48h EC_{10}	38; 50 mg/L	
(growth rate + biomass)	48h EC_{50}	110; 220 mg/L	(9152)
Selenastrum capricornutum	96h EC_{50}	12 mg/L	(9147)
	5d EC_{50}	280 mg/L	(9150)
Skeletonema costatum	5d EC_{50}	203 mg/L	(9150)
algae *(Microcystis aeruginosa):*	8d EC_0	120 mg/L	(329)
green algae *(Scenedesmus quadricauda):*	7d EC_0	>390 mg/L	(1900)
protozoa *(Entosiphon sulcatum):*	72h EC_0	>390 mg/L	(1900)
protozoa (*Uronema parduczi* Chatton-Lwoff):	EC_0	>392 mg/L	(1901)



(8359) *CAS* 2008-58-4

A. PROPERTIES: molecular weight 190.03; melting point 198–200°C.

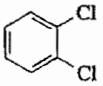
D. BIOLOGICAL EFFECTS:

(10085) (10087) ALGAE: *Chlorella fusca* BCF (wet wt): 3 (2659)

o-dichlorobenzene (1,2-dichlorobenzene)

(9872)

(10086)



$C_6H_4Cl_2$

CAS 95-50-1

(8899) *USES:* manufacture of 3,4-dichloro-aniline; solvent; dye mfg.; fumigant and insecticide; metal polishes; industrial odor control; technical grade contains *p*-dichlorobenzene (17%) and *m*-dichlorobenzene (2%).

(2696) A. PROPERTIES: colorless liquid; molecular weight 147.01; melting point –16.7/18°C; boiling point 179°C; vapor pressure 1 mm at 20°C, 1.5 mm at 25°C, 1.9 mm at 30°C; vapor density 5.07; d 1.3 at 20/4°C; solubility 100 mg/L at 20°C, 145 mg/L at 25°C; saturation concentration in air 8.0 g/m^3 at 20°C, 15 g/m^3 at 30°C; log P_{oct} 3.38; log H -1.00 at 25°C, 145 Pa m$_3$/mol at 10 °C, 165 Pa m$_3$/mol at 15 °C, 170 Pa m$_3$/mol at 20 °C, 159 Pa m$_3$/mol at 25 °C, 240 Pa m$_3$/mol at 30 °C (measured values).

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.116 ppm, 1 ppm = 6.01 mg/m^3.

Odor: recognition: 0.12 mg/m^3. (610)
T.O.C.: avg 50 ppm = 305 mg/m^3 (211, 279)
300 mg/m^3 (57, 291)

O.I. at 20°C = 26 (316)

Photochemical reactions: $t_{1/2}$: 27; 38; 53 d, based on reactions with OH°(calculated). (8967, 8968, 8969)

Manmade sources: in 4 municipal landfill gases in Southern Finland (1989–90 data):
avg < 0.01–0.2 mg/m^3, max 0.4 mg/m^3. (2605)

Incinerability:
Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 970°C.
Thermal stability ranking of hazardous organic compounds: rank 23 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

C. WATER AND SOIL POLLUTION FACTORS:

(2709) *Evaporation:*
50% evaporation from ponds into the atmosphere within 15 hours. (8972)
50% evaporation from solution at depth of 0.75 and 1.6 cm respectively: 1.2 and 2.5 minutes. (8973)
50% evaporation from 0.05 µg/L solution of Rhine water slowly stirred: 4 hours
90% evaporation from 0.05 µg/L solution of Rhine water slowly stirred: 24 hours (8976)

Indirect photolysis: at a depth of 8 cm beneath the surface of the river Goldbach 440 m above sea level under cloudless sky: $t_{1/2}$: 13 d (10h sunshine/d). (8970)

Reduction of amenities:
adverse taste in fish: <0.25 mg/L water (41)
T.O.C. = 0.01 mg/L (225, 903)

Water quality:

in river Maas (the Netherlands): average in 1973: 0.13 µg/L (*o*- + *p*-isomer) (342)
in Delaware River (U.S.A.): conc. range: winter: 0.4 ppb (n.s.i.) summer: n.d. (1051)
in Zurich lake: at surface: 16 ppt; at 30-m depth: 26 ppt (n.s.i.)
in tap water (Zurich): 4 ppt (n.s.i.) (513)

In rivers in U.K. (1986): 139 samples from 70 river sites yielded 37 positive values (detect. limit: 0.1 µg/L): median of positive values: 0.5 µg/L; maximum: 5.7 µg/L. (2711)
Waste water treatment: degradation by *Pseudomonas:* at 200 mg/L.
parent: 100% ring disruption in 72 h
mutant: 100% ring disruption in 26 h (152)

Degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.7 mg/L: 50% removal in less than 4 d; 66% removal in 32 d. The removal must be attributed to a chemical conversion or physical removal process other than sorption. (2653)

Water treatment:

initial concentration, µg/L	*treatment method*	*% removal*
501	river bank filtration	21
2,980	river bank filtration	45*
810	river bank filtration	44*
810	ozonization	83*
	slow filtration	97

* sum of isomers

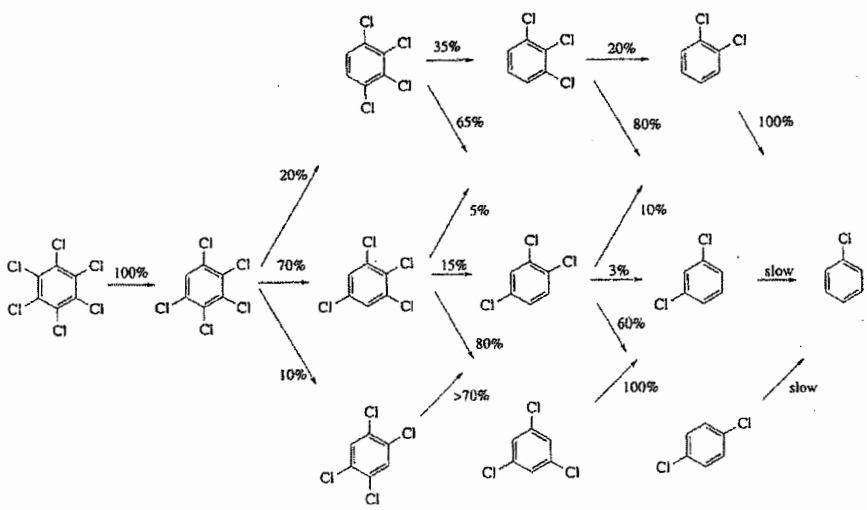
(2915)

Impact on biodegradation processes:
activated sludge respiration inhib. EC_{50}: >100 mg/L (2624)

Degradation in soil: disappearance in soil at 100 mg/kg and 20°C under aerobic laboratory conditions: $t_{1/2}$: 4.0 d; confidence limits: 3.0–6.1 d. (2366)
Calculated half-life in nonpolluted anaerobic aquifer at varying organic carbon contents (n.s.i.):

organic carbon content	1%	0.1%	0.01%	0.001%
average $t_{1/2}$	1,345 years	3,122 years	17,636 years	2,513 ages

(2695)
Biodegradation half-lives in nonadapted aerobic subsoil: sand Ontario: 250 d. (2695)
Reductive dechlorination in sediment under sulfate reducing conditions at 25 °C: half life period assuming peudo first order kinetics: 37 d. (7041)



Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

(342) *Mobility in the soil: soil sorption:* K_{oc}: 0.02-250; 286-4654; 383 at pH 6.3; 830 (8970, 8971, 2597)

Manmade sources:
Göteborg (Sweden) sew. works 1989–1991: infl.: n.d.; effl.: n.d. (2787)
(1051) anaerob. digest. sew. sludge from municipal area U.K. 1989: mean: 56 µg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area U.K. 1990:
(513) mean: 2,370 µg/kg (2688)
In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 (7000)
(2711) sludges ranged from 0.010 to 0,42 mg/kg dw.; mean: 0.13 mg/kg dw; mean value of sludge compost: ND.

Occurrence in sewage sludges, NW England 1989:

urban	mean	168 µg/kg dry wt	
(152)	SD	83 µg/kg dry wt	
urban/industrial	mean	1,870 µg/kg dry wt	
(2653)	SD	1,640 µg/kg dry wt	(2953)

Drinking water treatment plants where pure chlorine is used for disinfection in the Netherlands: jan-march 1994 (ng/L):

Pumpstation	Enschede	Andijk	Berenplaat	Kralingen	
raw water (intake)	< 80	< 80	< 80	< 80	
after rapid filtration	< 80	384	146	< 80	
after activated carbon		< 80		< 80	
rein water (effluent)	241	< 80	860	194	(7060)

Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
domestic sewage addapted	Closed Bottle Test	4 mg/L	20 d	58% ThOD	(8970)
(2915) A.S.	Modified MITI Test	100 mg/L	20 d	0% ThOD	(8977)

(2624) D. BIOLOGICAL EFFECTS:

(2366) *Residues:*
In Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 7.1 mg/kg of organic carbon
suspended sediments: not detected mg/kg of organic carbon
water: 9 ng/L
In catfish: Bayou d'Inde industrial outfall: 0.11 mg/kg of lipid
junction of Bayou d'Inde and Calcasieu River: 0.06 mg/kg of lipid
(2695) Lake Charles: not detect. mg/kg of lipid
(2695)
(7041)

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Cyprinus carpio	10	56 d	90-260	total body	(8977)
	100	56 d	150-230	total body	(8977)
Atlantic croakers			8700	lipid	
blue crabs			28,800	lipid	
spotted sea trout			6200	lipid	
blue catfish			6600	lipid	
rainbow trout			3,300-6,300	lipid	(2646)
Lepomis macrochirus	7.89	14 d	89*		(2602)
fathead minnow			89		(2606)

* half-life in tissues: <1 d

Biouptake by Oligochaete worms Tubifex tubifex *and* Limnodrilus hoffmeisteri: worm/sediment accumulation (2618)
factor after 79 d at 8°C and 0.23 mg/kg sedment: 0.2; $t_{1/2}$ in worm: <5 d.
Toxicity to microorganisms: act. sludge respiration inhib. EC_{50}: >100 mg/L (2624)
marine plankton: growth was stopped at 13 ppm (360)

BACTERIA

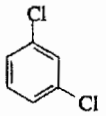
bacteria (*Pseudomonas putida*)	16h EC_0	15 mg/L	(1900)
aerobic heterotrophic culture inhibition of respiration	315h EC_{50}	910 mg/L	(8979)
Nitrosomonas inhibition of N-oxidation	24h EC_{50}	47 mg/L	(8979)
Pseudomonas fluorescens	24h EC_0	250 mg/L	(8980)
Photobacterium phosphoreum	5min EC_{50}	2.7 mg/L	(8979)
methanogenic bacteria inhibition of gas production	48h IC_{50}	150 mg/L	(8979)

	96h LC_{50},S	5.6 mg/L	(2697)
Brachydanio rerio	96h LC_{50}	5.2 mg/L	
	14d NOEC	0.37 mg/L	(8978)
Salmo gardneri	96h LC_{50}	1.6 mg/L	(8970)
	48h LC_{50}	2.3 mg/L	(8970)
Cyprinodon variegatus	96h LC_{50}	9.7 mg/L	(8970)
Leuciscus idus	48h LC_{50}	29 mg/L	(8970)
Oryzias latipes	48h LC_{50}	10 mg/L	(8977)
Pimephales promelas	96h LC_{50}	5.8 mg/L	(8970)

MAMMALS:

rat	oral LD_{50}	500; 2,138 mg/kg body wt

m-dichlorobenzene (1,3-dichlorobenzene)



$C_6H_4Cl_2$

CAS 541-73-1

USES AND FORMULATIONS: impurities in technical product:

1,4-dichlorobenzene	<3% wt.
1,2-dichlorobenzene	<1% wt.
chlorobenzene	<0.5% wt.

A. PROPERTIES: molecular weight 147.01; melting point –24.8°C; boiling point 172°C; d 1.29 at 20/4°C; vp: 0.00302 atm at 20°C, 1.8 hPa at 20°C; solubility 123 mg/L at 25°C, 100 mg/L, 110 mg/L, 131 mg/L at 20°C, 124 mg/L, 133 mg/L, 134 mg/L, 143 mg/L at 25°C, 200 mg/L at 60°C; 69 mg/L at 22°C; log P_{oct} 3.38/3.44, 3.55 at 19°C; 3.44 at 20°C; 3.6 at 22°C; 3.38; 3.44 at 25°C; 3.48 at 28°C (all measured values); log H -0.72 at 25°C.

B. AIR POLLUTION FACTORS:

Photochemical reactions: $t_{1/2}$: 16d; 16d; 37 d, based on reactions with $OH^{\bullet}$(calculated). (8073, 8074, 8075)

Manmade sources: in 4 municipal landfill gases in Southern Finland (1989–1990 data): avg <0.01–0.17, max 0.3 mg/m^3. (2605)

Incinerability:
Temperature for 99% destruction at 2.0 sec. residence time under oxygen-starved reaction conditions: 960°C.
Thermal stability ranking of hazardous organic compounds: rank 25 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

Ambient air quality: indoor/outdoor glc's winter 1981–1982 and 1982–1983 the Netherlands:
µg/m^3

	median	*maximum*	
pre-war homes	<0.6	6	
post-war homes	<0.6	9	
homes <6 years old	<0.6	6	
outdoors	<0.6	<0.6	(2668)

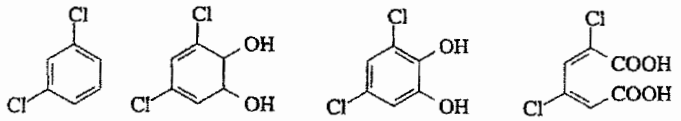
C. WATER AND SOIL POLLUTION FACTORS:

Manmade sources:
anaerob. digest. sew. sludge from municipal area U.K., 1989: mean: 7 µg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area U.K., 1990:
mean: 333 µg/kg (2688)
Göteborg (Sweden) sew. works 1989–1991: infl.: n.d.; eff.: n.d. (2787)
In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 sludges ranged from 0.003 to 0.077 mg/kg dw.; mean: 0.025 mg/kg dw;mean value of sludge compost: ND. (7000)

Surface water quality:
In Bayou d'Inde, LA, U.S.A., near industrial outfall:
bottom sediments: 101 mg/kg of organic carbon
suspended sediments: 0.98 mg/kg of organic carbon
water: 48 ng/L
In rivers in U.K. (1986): 139 samples from 70 river sites yielded 35 positive values (detection limit: 0.1 µg/L): median of positive values: 0.6 µg/L; maximum: 5.7 µg/L. (2711)

Waste water treatment:
degradation by *Pseudomonas:* at 200 mg/L at 30°C
parent: 100% ring disruption in 96 h
mutant: 100% ring disruption in 28 h (152)

Degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.7 mg/L: 50% removal in less than 4 d; 77% removal in 32 d. Biodegradation may have been the mechanism of removal for part or all of the reductions observed.
Reduction of amenities: T.O.C. = 0.02 mg/L. (225, 903)
Soil sorption: log K_{oc}: 3.23. (2597)
Degradation in soil:
Biodegradation by Alcaligenes *sp. as the sole carbon and energy source according to the following pathway:*

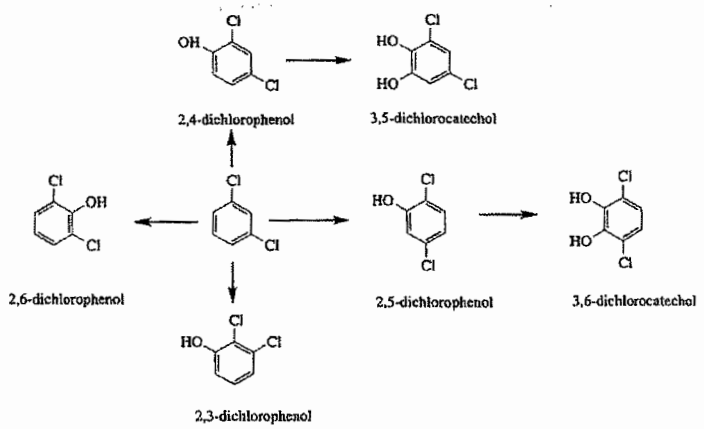


3,5-dichloro-*cis*-1,2-dihydroxycyclo-*hex*-3,5-diene | 3,5-dichlorocatechol | 2,4-dichloromuconat

(2615)

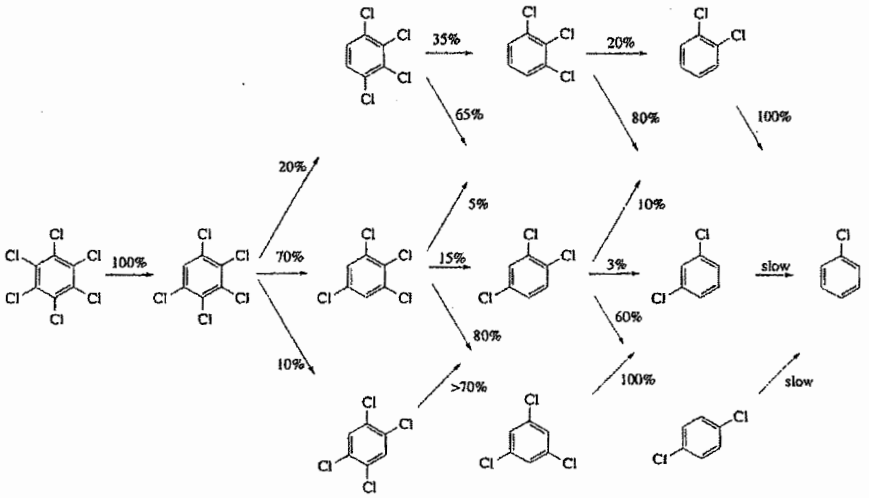
Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
	Repetitive Die-away Test		28 d	0% ThOD	(8085)
mixed culture		200 mg/L	4 d	100% product	(8086)
domestic A.S.	1ste subculture Closed Bottle Test	5 mg/L	7 d	69% product	
domestic A.S.	2nd subculture	5 mg/L	7 d	31% product	
domestic A.S.	3rd subculture	5 mg/L	7 d	33% product	(8077, 8078)
clarifier sludge	glass beads column	9.8 µg/L	20 min RT	15-22% product	
	after 9 months	9.8 µg/L	20 min RT	34-71% product	(8082; 8083)
adapted soil micro-organisms	in aerobic soil column	15-150 µg/L	0 d	0% product	
	after 80 d inocculation			95% product	(8089, 8090, 8091)
	under anaerobic conditions			0% product	(8092)
Methanogenic bacteria	in glass bead column	10 µg/L	2 dRT	0-15% product	(8082)
anaerobic sludge		710 µg/L	1 d	16% product	
			2 d	34% product	
			4 d	53% product	
			8 d	62% product	
			16 d	65% product	(8093)



Aerobic biodegradation by mixed culture of benzene adapted soil micro-organisms and Pseudomonas sp.: metabolites detected after 20 d incubation. (8087, 8088)

Reductive dechlorination in sediment under sulfate reducing conditions at 25°C: half life period assuming peudo first order kinetics: 433 d. (7041)



Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

Water treatment:

method	*concentration*	*duration*	*elimination results*	
activated carbon column	9.9 µg/L	60 min retention time	95% product	(8084)

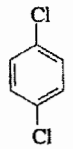
D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Fishes: *Lepomis macrochirus*		30 d	98	total body	
Poecilia reticulata		48 hours	6918	lipid	
Atlantic croakers					
bluegill sunfish (*Lepomis macrochirus*)	107		66*		(2602)
spotted sea trout			1780	lipid	
blue catfish			2510	lipid	
rainbow			5,010-1,0500	lipid	(2646)
Crabs: blue crabs			3980	lipid	

* half-life in tissues: <1 d

33d LOEC	2.3 mg/L	
33d MATC	1.5 mg/L	(8104, 8105)

p-dichlorobenzene (1,4-dichlorobenzene)



$C_6H_4Cl_2$

CAS 106-46-7

MANUFACTURING SOURCE: organic chemical industry. (347)

USERS AND FORMULATION: mfg. moth repellants; mfg. air deodorizers; mfg. dyes and intermediates; pharmaceuticals mfg.; soil fumigant; pesticide. (347)

A. PROPERTIES: colorless or white crystals; molecular weight 147.01; melting point 53°C; boiling point 173.4°C; vapor pressure 0.6 mm at 20°C, 1.8 mm at 30°C; vapor density 5.07; d 1.46 at 20/4°C; solubility 49 mg/L at 22°C, 79 mg/L at 25°C; saturation concentration in air 4.8 g/m^3 at 20°C, 14 g/m^3 at 30°C; log P_{oct} 3.39 at 20°C; log H −1.10 at 25°C.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.166 ppm, 1 ppm = 6.01 mg/m^3.

Odor: characteristics: quality: very distinctive aromatic odor; T.O.C.: 15–30 ppm; O.I. at 20°C = 26. (211, 316)
Manmade sources: in 4 municipal landfill gases in Southern Finland (1989–1990 data):
avg <0.05–0.18, max 0.3 mg/m^3. (2605)

Incinerability: thermal stability ranking of hazardous organic compounds: rank 21 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)
Ambient air quality:
Indoor/outdoor glc's winter 1981–1982 and 1982–1983 the Netherlands:

	median	*maximum* (μg/m^3)
pre-war homes	<0.6	299
post-war homes	2	138
homes <6 years old	<0.6	240
outdoors	<0.6	<0.6

(2668)

Inside and outside 15 living rooms in Northern Italy (1983–1984):

4–7 d averages	*lowest*	*mean*	*highest value (all in μg/m^3)*
indoor	<5	55	230
outdoor	<2	<5	4

(2756)

C. WATER POLLUTION FACTORS:

Reduction of amenities:
T.O.C. = 0.03 mg/L (225, 903)
= 0.0003 mg/kg (894)

Water quality:
In river Maas at Eysden (the Netherlands) in 1976:
median: 0.1 μg/L; range: n.d.–3.5 μg/L.
In river Maas at Keizersveer (Netherlands) in 1976:
median: n.d.; range: n.d.–0.4 μg/L. (1368)
In Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 82 mg/kg of organic carbon
suspended sediments: 1.2 mg/kg of organic carbon
water: 74 ng/L.
In rivers in U.K. (1986): 139 samples from 70 river sites yielded 29 positive values (detection limit: 0.1 μg/L): median of positive values: 0.7 μg/L; maximum: 13 μg/L.

(2711)

Waste water treatment:
degradation by *Pseudomonas:* 200 mg/L at 30°C

parent:	100% ring disruption in 92 h
mutant:	100% ring disruption in 25 h

(152)

Degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.7 mg/L: 50% removal in 18–16 d; 80% removal in 32 d. Biodegradation may have been the mechanism of removal for part or all of the reductions observed. (2653)
Removal in an activated sludge aeration basin: 19% stripped into the air, 55% biotransformed. (2793)

Water treatment:

initial concentration, µg/L	*treatment method*	*% removal*
10–10,000	river bank filtration	80
472	river bank filtration	53
2980	river bank filtration	45*
810	river bank filtration	44*
810	ozonization	83*
	activated carbon	90–100
	slow filtration	97

* sum of isomers (2915)

Soil sorption: log K_{oc}: 3.22. (2597)

K_{oc}:	for Fullerton soil, 0.06% OC	850
	for Apison soil, 0.11% OC	665
	for Dormont soil, 1.2% OC	280

(2599)

Manmade sources:
anaerob. digest. sew. sludge from municipal area U.K., 1989: mean: 1,020 µg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area U.K., 1990: mean: 957 µg/kg. (2688)
Göteborg (Sweden) sew. works 1989–1991: infl.: 0–0.5 µg/L; effl.: n.d. (2787)
In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 sludges ranged from 0.033 to 0.87 mg/kg dw.; mean: 0.49 mg/kg dw; mean value of sludge compost: 0.0022 mg/kg dw. (7000)
drinking water treatment plants where pure chlorine is used for disinfection in the Netherlands: jan-march 1994 (ng/L):

Pumpstation	Enschede	Andijk	Berenplaat	Kralingen
raw water (intake)	< 80	< 80	< 80	< 80
after rapid filtration	< 80	611	369	< 80
after activated carbon		< 80		< 80
rein water (effluent)	159	< 80	1293	< 80

(7060)

Occurrence in sewage sludges, NW England, 1989:

urban	mean:	1,090 µg/kg dry wt
	SD:	579 µg/kg dry wt
urban/industrial	mean:	1,620 µg/kg dry wt
	SD:	455 µg/kg dry wt

(2953)

Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
domestic sewage	Closed Bottle Test	28 d		67% ThOD	(8426)
industrial A.S. non-adapted	Modified Zahn-Wellens Test	5 d		5% DOC	
		10 d		15% DOC	
		15 d		20% DOC	
		20 d		20% DOC	(8427)
A.S.	Confirmatory Test			97%*	(8426)

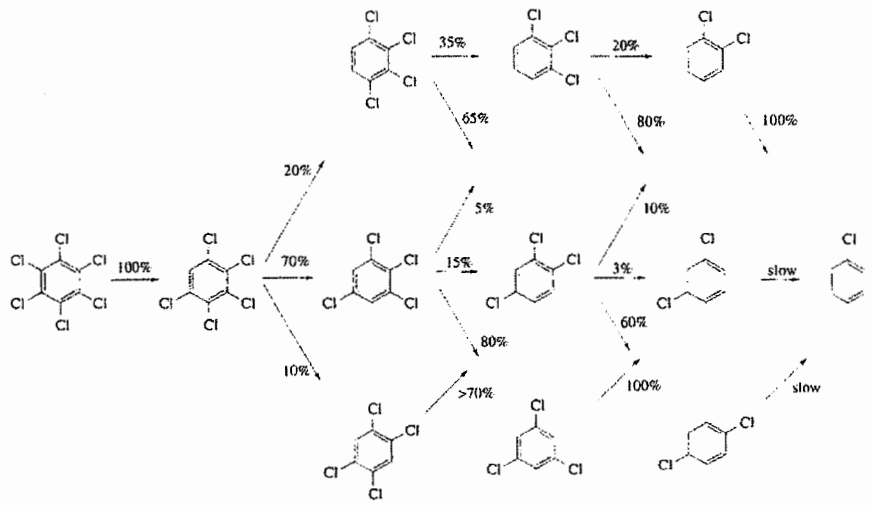
* 67% elimination related to stripping

(2711) Reductive dechlorination in sediment under sulfate reducing conditions at 25 °C: half life period assuming peudo first order kinetics: 385 d. (7041)

(152)

(2653)

(2793)



(2915)

Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

(2597)

D. BIOLOGICAL EFFECTS:

(2599)

Bioaccumulation:	Concentration µg/L	exposure period	BCF	organ/tissue	
bacteria (*Sidero capsa treubii*)			20		(1833)
guppies (*Poecilia reticulata*):			1,800	lipid	
trout (*Salmo gairdneri*):			214		(193)
rainbow trout	0.028-0.067		510-890		(2399, 2400)
Atlantic croakers			8130		
blue crabs			33,900		
spotted sea trout			12,300		
blue catfish			3200		(2646)
rainbow trout			400-9100		(2646)
bluegill sunfish (*Lepomis macrochirus*)	10.1	14 d	60*		(2602)
fathead minnow			112		
bluegill			60		
guppy			91		(2606)

(2688)
(2787)
(7000)
ng/L):
(7060)

* half-life tissues: <1 d

in catfish: Bayou d'Inde industrial outfall:	0.47 mg/kg of lipid	
junction of Bayou d'Inde and Calcasieu River:	0.24 mg/kg of lipid	
Lake Charles:	0.17 mg/kg of lipid	(2646)

(2953)

Biouptake by Oligochaete worms Tubifex tubifex *and* Limnodrilus hoffmeisteri: worm/sediment accumulation factor after 79 d at 8°C and 0.37 mg/kg sediment: 0.2 (2618)

(8426) BACTERIA:

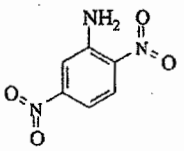
OECD 209 closed system	EC_{50}	>80 mg/L	(2624)
A.S. oxygen consumption inhibition	3h EC_{50}	>10,000 mg/L	(8435)
primary municipal sludge (ETAD Fermentation tube method)	24h EC_0	15 mg/L	(8427)
Pseudomonas fluorescens	24h EC_0	500 mg/L	(8435)
Nitrosomonas sp. (inhib.of N oxidation)	24h IC_{50}	86 mg/L	(8433)

(8427)
(8426)

952 2,5-dinitroaniline

BACTERIA:			
Photobacterium phosphoreum Microtox test	30min EC_{50}	48.2 mg/L	(8899)
ALGAE:			
Tetrahymena pyriformis: growth inhibition at 27°C	48 EC_{50}	35 mg/L	(2704)
Scenedesmus subspicatus: inhib. of fluorescence	IC_{10}	0.79 mg/L	
growth inhib.	IC_{10}	0.055 mg/L	(2698)
RubisCo test: inhib. of enzym. activity of Ribulose-P2-carboxylase in protoplasts	IC_{10}	0.92 mg/L	
Oxygen test: inhib. of oxygen production of protoplasts	IC_{10}	7.3 mg/L	(2698)
CRUSTACEANS:			
Daphnia magna	24h EC_{50}	12.0 mg/L	
	48h EC_{50}	9.6 mg/L	(9910)
FISHES:			
Pimephales promelas:	30-35d LC_{50}	235 mg/L	(2704)
fathead minnow	96h LC_{50}	14.2 mg/L	(7643)
MAMMALS:			
mouse	oral LD_{50}	370 mg/kg bw	(9789)
guinea pig	oral LD_{50}	1,050 mg/kg bw	(10187)

2,5-dinitroaniline



$(NO_2)_2C_6H_3NH_2$

$C_6H_5N_3O_4$

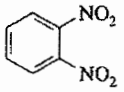
A. PROPERTIES: molecular weight 183.12.

C. WATER AND SOIL POLLUTION FACTORS: constituent of condensate water of TNT manufacturing process.

D. BIOLOGICAL EFFECTS:

fathead minnow	96h LC_{50}	21 mg/L	(2627)
water flea	48h LC_{50}	13.8–15.4 mg/L	(2627)

o-dinitrobenzene



$C_6H_4(NO_2)_2$

$C_6H_4N_2O_4$

(8899) *CAS* 528-29-0

USE: Analytical reagent. Manufacture of dyestuffs.

(2704) A. PROPERTIES: colorless to yellowish needles; molecular weight 168.11; melting point 118°C; boiling point 319°C at 773 mm; vapor density 5.79; d 1.56 at 17/4°C; solubility 100 mg/L (cold), 3,800 mg/L at 100°C; log P_{oct} 1.58.

(2698) B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.14 ppm, 1 ppm = 6.99 mg/m^3.

Incinerability: thermal stability ranking of hazardous organic compounds: rank 158 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)
Photochemical reactions: $t_{1/2}$: 14-15 h, based on reactions with OH°(calculated). (8481)

(2698) C. WATER POLLUTION FACTORS:

Reduction of amenities: organoleptic limit: 0.5 mg/L (n.s.i.). (181)
Biodegradation: decomposition by a soil microflora: period: >64 d. (176)

(9910) Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
(2704) sewage sludge	aerobic		28 d	25%	
(7643) sewage sludge	anaerobic		14 d	100%	(7894)

Mobility in soil: K_{oc}: 1.47.

(9789) (10187) D. BIOLOGICAL EFFECTS:

BACTERIA:

Photobacterium phosphoreum Microtox test	30min EC_{50}	5.3 mg/L	(8899)

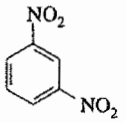
CRUSTACEANS:

Daphnia magna	48h EC_{50}	2.9 mg/L	(7914)

FISHES:

guppy	14d LC_{50}	1.1 mg/L	(7902)

m-dinitrobenzene (1,3-dinitrobenzene; 1,3-DNB)



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$C_6H_4(NO_2)_2$

(2627) (2627) $C_6H_4N_2O_4$

CAS 99-65-0

MANMADE SOURCES: Constituent of condensate water of TNT manufacturing process.

USES AND FORMULATIONS: Analytical reagent. Catalyst. Corrosion inhibitor.

IMPURITIES: 1,2-dinotrobenzene <1,2%; 1,4-dinitrobenzene <0.2%.

A. PROPERTIES: colorless to yellowish needles; molecular weight 168.11; melting point 89.8°C; boiling point 300–02°C at 770 mm; vapor pressure 1.93 ×10^{-4} torr at 25°C, <0.0038 hPa at 20°C, <0.0058 hPa at 25°C, 0.1 hPa at 80°C; 0.5 hPa at 100°C; density 1.571 at 0/4°C; solubility 469 mg/L at 15°C, 3,200 mg/L at 100°C, 530 mg/L at 20°C, 533 mg/L at 25°C, 654 mg/L at 30°C; log P_{oct} 1.49; log H -5.4 at 20°C.

B. AIR POLLUTION FACTORS:

Incinerability: thermal stability ranking of hazardous organic compounds: rank 154 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

Photochemical reactions: $t_{1/2}$: 14– 15 h; 520 d, based on reactions with OH°(calculated). (7892, 8481)

C. WATER AND SOIL POLLUTION FACTORS

Biodegradation: decomposition by a soil microflora in >64 d; (176)

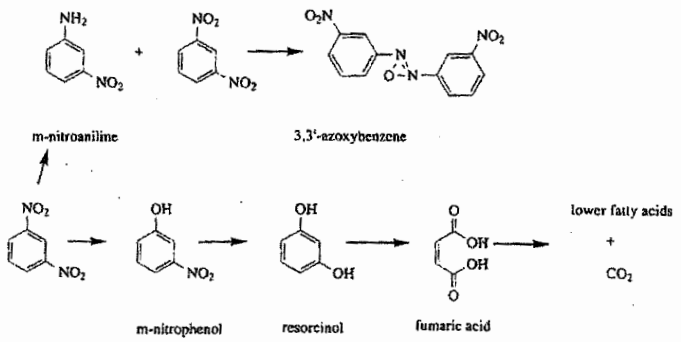
Adapted A.S. at 20°C—product is sole carbon source: 0% COD removal after 20 d. (327)

BIODEGRADATION

Inoculum	*Method*	*Concentration*	*Duration*	*Elimination results*	
Municipal nonadapted A.S.	Anaerobic at 29°C in the dark	10 mg/L	28 d	>40% product*	(7894)
Industrial A.S.	Modified Zahn-Wellens test	430 mg/L	15 d	0% DOC	(7893)
Azotobacter agilis	2-stage water treatment unit	136 mg/L	36 h	98% product	(7895)
Adapted river water		5 mg/L	15 d	>99% product**	(7896)
Sewage sludge	Aerobic		28 d	40%	
Sewage sludge	Anaerobic		28 d	85%	(7894)

* mg/L nitroaniline was detected as metabolite after 14 d; ** after lag period of 10 d.

Adapted yeast, fungi, and bacteria of the following species were able to degrade 100–150 mg/L 1,3-dinitrobenzene as the sole carbon source: *Candida, Aspergillus, Pseudomonas, Acinetobacter, Arthrobacter, Streptomyces, Micrococcus, Staphylococcus, Micromonospora, Vibrio, Klebsiella, Bacillus*. A number of metabolites were detected (see below).



Metabolites identified in a number of biodegradation experiments. (7894, 7897, 7898, 7899, 7900, 7901)

Soil sorption: log K_{oc}: 1.56.

D. BIOLOGICAL EFFECTS:

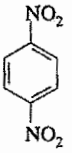
Bioaccumulation	*Concentration µg/L*	*Exposure period*	*BCF*	*Organ/tissue*	
FISHES: trout			8.5	Muscle	(8801)
Poecilia reticulata	770	3 d	4.5–7.5	Total body	
			74	Lipid	(7902)

BACTERIA:

Pseudomonas putida	16 h EC_0	14 mg/L	(1900)
Anaerobic municipal sludge gas production	24 h EC_0	30 mg/L	(7893)
Mycobacterium tuberculosis var. *hominis* cell multiplication	14 d EC_{10}	5 mg/L	(7917)
Chilomonas paramecium	48 h LC_{10}	1.1 mg/L	(7916)
Photobacterium phosphoreum	15 min EC_{50}	40 mg/L	(7914)
Streptococcus sp.	48 h LC_{10}	33 mg/L	(7917)
Pseudomonas fluorescens	17 h EC_{10}	5 mg/L	(8696)
Photobacterium phosphoreum Microtox test	30 min EC_{50}	26.6 mg/L	(8899)

	60 d LOEC	0.84 mg/L	
	60 d NOEC	0.44 mg/L	(8693)
Silver carp	96 h LC_{50}	9.9 mg/L	(10188)
MAMMALS:			
Rat	Oral LD_{50}	42 mg/kg bw	(10189)

p-dinitrobenzene (1,4-dinitrobenzene)



$C_6H_4(NO_2)_2$

$C_6H_4N_2O_4$

CAS 100-25-4

USES: Corrosion inhibitor. Cross-linking agent. Chemical intermediate.

A. PROPERTIES: colorless to yellowish needles; molecular weight 168.11; melting point 173°C; boiling point 299°C at 777 mm (sublimes); vapor pressure < 1 mm Hg at 20°C; vapor density 5.8; density 1.6 at 20/4°C; solubility 800 mg/L at 20°C; 1,800 mg/L at 100°C; log P_{oct} 1.46/1.49.

B. AIR POLLUTION FACTORS:

Incinerability: thermal stability ranking of hazardous organic compounds: rank 158 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)
Photochemical reactions: $t_{1/2}$: 14-15 hours, based on reactions with OH°(calculated). (8481)

C. WATER POLLUTION FACTORS:

Biodegradation:
decomposition by a soil microflora in >64 d. (176)
adapted A.S. at 20°C-product is sole carbon source: 0% COD removal after 20 d.

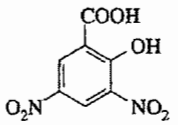
Mobility in soils: log Koc: 1.46

D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Fishes: trout			0.91	muscle	(8801)

BACTERIA:			
Photobacterium phosphoreum Microtox test	30 min EC_{50}	0.095 mg/L	(8899)
ALGAE:			
Tetrahymena pyriformis: growth inhibition	48 EC_{50}	8.4 mg/L	(2704)
CRUSTACEANS:			
Daphnia magna	48h EC_{50}	1.2 mg/L	(7914)
FISHES:			
Pimephales promelas:	30-35 d LC_{50},F	170 mg/L	(2704)
fathead minnow	96h LC_{50}	0.6 mg/L	(7644)
guppy	14d LC_{50}	0.36 mg/L	(7902)

(327)
(998)



$(NO_2)_2C_6H_2(OH)COOH$

(2624)

$C_7H_4N_2O_7$

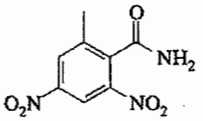
(2704) *CAS* 609-99-4

A. PROPERTIES: molecular weight 228.12; melting point 169–172°C.

(2704) C. WATER POLLUTION FACTORS:

Biodegradation: adapted A.S. at 20°C—product is sole carbon source: 0% COD removal after 20 d. (327)

3,5-dinitro-*o*-toluamide (zoalene)



$(NO_2)_2C_6H_2(CH_3)CONH_2$

$C_8H_7N_3O_5$

USE: coccidiostat; permissible food additive.

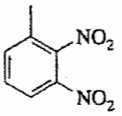
A. PROPERTIES: yellowish solid; melting point 177°C; solubility 1,000 ppm.

D. BIOLOGICAL EFFECTS:

(2624)

FISHES:			
guppy	48h LC_{50},S	>200 mg/L at 24°C	
rainbow trout	48h LC_{50},S	>200 mg/L at 15°C	(446)

2,3-dinitrotoluene (1-methyl-2,3-dinitrobenzene; 2,3-DNT)



$CH_3C_6H_3(NO_2)_2$

lecomposes vapor

$C_7H_6N_2O_4$

CAS 602-01-7

USES: In the manufacture of explosives.

(292) A. PROPERTIES: molecular weight 182.14; melting point 59-61°C; log P_{oct} 2.0 (calculated).

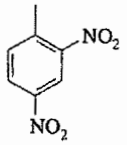
C. WATER AND SOIL POLLUTION FACTORS:

Manmade sources: constituent of condensate water of TNT manufacturing process.
Mobility in soil: K_{oc}: 290

D. BIOLOGICAL EFFECTS:

BACTERIA:			
Pseudomonas putida	16h EC_0	9 mg/L	(1900)
Photobacterium phosphoreum Microtox test	15min EC_{50}	6.03 mg/L	(8899)
ALGAE:			
Microcystis aeruginosa	8d EC_0	0.22 mg/L	(329)
green algae (*Scenedesmus quadricauda*)	7d EC_0	0.83 mg/L	(1900)
Selenastrum capricornutum	96h EC_{50}	1.37-1.62 mg/L	(10195)
PROTOZOANS:			
protozoa (*Entosiphon sulcatum*)	72h EC_0	5.9 mg/L	(1900)
protozoa (*Uronema parduczi* Chatton-Lwoff)	EC_0	1.6 mg/L	(1901)
CRUSTACEANS:			
water flea	48h LC_{50}	4.7 mg/L	(2627)
Daphnia magna	48h EC_{50}	0.66 mg/L	
FISHES:			
fathead minnow	96h LC_{50}	1.8 mg/L	(2627)
bluegill sunfish, sheephead minnow	96h LC_{50}	0.33-2.28 mg/L	(10195)
MAMMALS:			
rat, mouse	oral LD_{50}	910-1,100 mg/kg bw	(9710, 9836)

2,4-dinitrotoluene (1-methyl-2,4-dinitrobenzene; 2,4-DNT)



$CH_3C_6H_3(NO_2)_2$

$C_7H_6N_2O_4$

CAS 121-14-2

USES: Intermediate in the manufacture of toluene diisocyanate and polyurethanes; ingredient in the manufacture of dyes and military and commercial explosives.

OCCURRENCE: In waste waters and soils at TNT production sites.

A. PROPERTIES: yellow needles; molecular weight 182.13; melting point 70°C; boiling point 300°C sl. decomposition; vapor density 6.27; vapor pressure 2.17×10^{-4} torr at 25°C, 8 x 10-5 hPa at 20°C; d 1.52 at 15°C; solubility 270 mg/L at 22°C, 166 mg/L at 20°C; log P_{oct} 1.98; H 0.088 Pa m^3/mol.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.13 ppm, 1 ppm = 7.57 mg/m^3.

Incinerability: thermal stability ranking of hazardous organic compounds: rank 168 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

C. WATER AND SOIL POLLUTION FACTORS

Manmade sources: constituent of condensate water of TNT manufacturing process: Göteborg (Sweden) sew. works 1989–1991: infl.: nd–0.5 µg/L; effl.: n.d. (2787)

(1900)
(8899)

Degradation:
Microbial degradation products include aminonitrotoluenes, nitrosonitrotoluenes, and dinitroazoxytoluenes. (2628)
Mineralization in natural waters at 1.0– 15 ppb at 25°C: after lag time of 2 d; complete mineralization was obtained after 5– 6 d. (2628)

(329)
(1900)

Maximum rates of mineralization in natural waters at 25°C after 2– 3-d incubation lag:

(10195)

conc., mg/L	*%/d*	*mg/L/d*	*% degraded*	
10	32.3	3.23	64	
0.1	10.7	0.0107	47	
0.01	10.9	0.0011	60	
0.004	10.4	0.0004	45	(2628)

(1900)
(1901)

Waste water treatment: activated carbon: at an effluent conc. of 1 mg/L, the equilibrium adsorptive capacities of virgin FS 300, virgin FS 400, and virgin powdered FS 300 (from Calgon) are 0.21, 0.30, and 0.25 g of DNT/g of C, respectively. Some of the adsorbed DNT is converted to its derivatives. The presence of 2,4-dinitrobenzoic acid, 2,4-dinitrobenzaldehyde, 2,4-dinitrobenzylalcohol, and 2,4-dinitrobenzoate indicates the occurrence of side-chain oxidation.

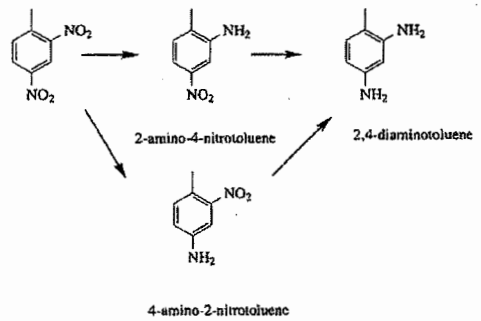
(2627)

BIODEGRADATION

Inoculum	*method*	*Concentration*	*duration*	*elimination results*	
River water	Sole C source	0.004– 10 mg/L	2– 3 d	45-64% $ThCO_2$	(8011)
Industrial A.S.	Zahn-Wellens test	60 mg/L	1 d	1% TOC	(8010)
White rot *Planerochaete chrysosporium*	As sole N source		24 d	34% $ThCO_2$	(8012)

(2627)
(10195)

(9710, 9836)

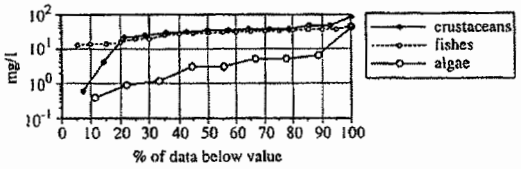


White rot *Planerochaete chrysosporium* degraded 2,4-DNT, as sole N source, after 24-d incubation. A few metabolites were identified. (8012)

Soil sorption: log K_{oc}: 2.40.

D. BIOLOGICAL EFFECTS:

acture of dyes and



ecomposition;
270 mg/L at 22°C,

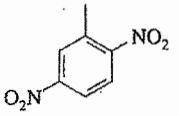
BACTERIA:

Pseudomonas putida	16 h EC_0	57 mg/L	(1900)

(cell multiplication inhibition test)	30 min NOEC	50 mg/L	(8007)
ALGAE:			
Microcystis aeruginosa	8 d EC_0	0.13 mg/L	(329)
Scenedesmus quadricauda	7 d EC_0	2.7 mg/L	(1900)
Tetrahymena pyriformis: growth inhib. at 27°C	48 h EC_{50}	42 mg/L	(2704)
Scenedesmus subspicatus	48 h EC_{10}	1.3– 1.9 mg/L	
(cell multiplication inhibition test)	48 h EC_{50}	3.0– 6.3 mg/L	(8009)
Selenastrum capricornutum	4 d EC_{37}	0.9 mg/L	
	4 d EC_{100}	24– 94 mg/L	(8007)
PROTOZOA:			
Entosiphon sulcatum	72 h EC_0	0.98 mg/L	(1900)
Uronema parduczi Chatton-Lwoff	EC_0	0.55 mg/L	(1901)
CRUSTACEANS:			
Water flea	48 h LC_{50}	47 mg/L	(2627)
Daphnia magna	24 h EC_0	10; 13 mg/L	
	24 h EC_{50}	22; 31; 38 mg/L	(8007, 8008)
	24 h EC_{100}	39 mg/L	(8007)
	48 h EC_{50}	30; 35; 38 mg/L	
	96 h EC_{50}	24 mg/L	
Reproduction rate	21d NOEC	< 0.5 mg/L	(8007)
WORMS:			
Lumbriculus variegatus	24 h LC_{50}	99 mg/L	
	48 h LC_{50}	>83 mg/L	
	96 h LC_{50}	47 mg/L	(8007)
FISHES:			
Pimephales promelas	30– 35 d LC_{50}-F	24 mg/L	(2704)
Fathead minnow	96 h LC_{50}	33 mg/L	(2627)
Lepomis macrochirus	96 h LC_{50}	13; 96 mg/L	(8007)
Pimephales promelas	96 h LC_{50}	28; 36 mg/L	(8007)
Salmo gairdneri	96 h LC_{50}	14; 14 mg/L	(8007)
Brachydanio rerio	96 h LC_0	24 mg/L	
	96 h LC_{100}	75 mg/L	(8007)
Leuciscus idus	96 h LC_0	24 mg/L	
	96 h LC_{100}	32 mg/L	(8007)

Lowest NOEC per species	µg/L	
Bacteriophyta	29,000	
Chlorophyta	320; 320; 560; 1,400	
Cyanophyta	65	
Euglenophyta	1,000	
Crysophyta	1,000	
Protozoa	490; 6,500	
Branchiopoda	130	
Pisces	1,000; 1,000; 1,000; 1,000; 3,200	(2906)

2,5-dinitrotoluene (2,5-DNT)



$CH_3C_6H_3(NO_2)_2$

(8007) $C_7H_6N_2O_4$

CAS 619-15-8

(329)
(1900)
(2704)

A. PROPERTIES: molecular weight 182.14.

C. WATER AND SOIL POLLUTION FACTORS: constituent of condensate water of TNT manufacturing process.

(8009)

D. BIOLOGICAL EFFECTS:

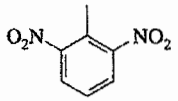
(8007)

CRUSTACEANS: water flea	48h LC_{50}	3.1 mg/L	(2627)
FISHES: fathead minnow	96h LC_{50}	1.3 mg/L	(2627)

(1900)
(1901)

2,6-dinitrotoluene (2,6-DNT)

(2627)



(8007, 8008)
(8007) $CH_3C_6H_3(NO_2)_2$

(8007) $C_7H_6N_2O_4$

CAS 606-20-2

USE: intermediate in the manufacture of toluene diisocyanate and polyurethanes, ingredient in the manufacture of dyes and military and commercial explosives.

(8007)

MANUFACTURING SOURCE: explosives mfg.; organic chemical industry. (347)

(2704)
(2627)
(8007)
(8007)
(8007)

USERS AND FORMULATION: mfg. TNT; urethane polymers, flexible and rigid foams and surface coatings, dyes; organic synthesis. (347)

A. PROPERTIES: molecular weight 182.14; melting point 64-66°C; boiling point 285°C; vapor pressure 5.67×10^{-4} torr at 25°C; density 1.54 at 15°C; solubility 208 mg/L at 25°C; log P_{oct} 1.89; log H –3.47 (measured).

(8007)

B. AIR POLLUTION FACTORS:

(8007)

Incinerability: thermal stability ranking of hazardous organic compounds: rank 168 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)
Photochemical reactions: $t_{1/2}$: 8h, based on reactions with OH°(calculated). (9677)

C. WATER AND SOIL POLLUTION FACTORS:

Odor threshold: 0.1 mg/L; detection: 0.05-1.0 mg/kg. (225, 903)
Manmade sources: constituent of condensate water of TNT manufacturing process: Göteborg (Sweden) sew. works 1989-1991: infl.: nd-0.5 μg/L; effl.: nd. (2787)
In Canadian municipal sludges and sludge compost: September 1993- February 1994: mean values of 11 sludges ranged from ND to 0.57 mg/kg dw.; mean: 0.07 mg/kg dw; mean value of sludge compost: ND. (7000)
(2906) *Soil sorption:* log K_{oc}: 1.89.
Degradation:
Microbial degradation products include aminonitrotoluenes, nitrosonitrotoluenes, and dinitroazoxytoluenes. (2628)
Mineralization in natural waters at 1.0–15 ppb at 25°C: after lag time of 2 to 5 d. Complete mineralization was obtained after 9 to 44 d. (2628)
Photolysis in water under sunlight: $t_{1/2}$: 17-24 h. (9707, 9708)
Adsorption capacity of activated carbon 145 g/kg carbon.
Maximum rates of mineralization in natural waters at 25°C after 2 to 3 d incubation lag:

conc., ppm	*%/d*	*mg/L/d*	*% degraded*
10	14.5	1.45	55

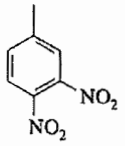
0.1	5.45	0.055	33	
0.01	—	0.00002	4	
0.004	—	0.000008	6	(2628)

D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
algal biomass				5225	(9706)

BACTERIA:			
Pseudomonas putida	16h EC_0	26 mg/L	
Photobacterium phosphoreum Microtox test	15min EC_{50}	2.9 mg/L	(9682)
Nitrosomonas nitrification	25d IC_{50}	180 mg/L	(9621)
methanogenic bacteria	50d IC_{50}	7.9 mg/L	(9621)
ALGAE:			
green algae (*Scenedesmus quadricauda*)	7d EC_0	12 mg/L	
protozoa (*Entosiphon sulcatum*)	72h EC_0	11 mg/L	(1900)
PROTOZOANS:			
Uronema parduczi Chatton-Lwoff	EC_0	23 mg/L	(1901)
CRUSTACEANS:			
water flea	48h LC_{50}	22 mg/L	(2627)
Daphnia magna	48h EC_{50}	34 mg/L	(7914)
FISHES: fathead minnow	96h LC_{50}	18 mg/L	(2627)
MAMMALS:			
rat, mouse	oral LD_{50}	180-620 mg/kg	(9709, 9710)

3,4-dinitrotoluene (3,4-DNT; 4-methyl-1,2-dinitrobenzene)



$CH_3C_6H_3(NO_2)_2$

$C_7H_6N_2O_4$

CAS 610-39-9

USE: Manufacture of dyestuffs and explosives.

A. PROPERTIES: molecular weight 182.14; melting point 54-57°C; density 1.26 at 111°C; log P_{oct} 2.0 (calculated).

B. AIR POLLUTION FACTORS:

Photochemical reactions: $t_{1/2}$: 8 hours, based on reactions with OH°(calculated). (8481)

C. WATER AND SOIL POLLUTION FACTORS

Manmade sources:: constituent of condensate water of TNT manufacturing process.

(2628)

D. BIOLOGICAL EFFECTS:

BACTERIA:			
Photobacterium phosphoreum Microtox test	15min EC_{50}	6.9 mg/L	(8899)
ALGAE:			
Chlorella pyrenoidosa	96h EC_{50}	0.75 mg/L	(7914)
CRUSTACEANS:			
water flea	48h LC_{50}	3.7 mg/L	(2627)
Daphnia magna	48h EC_{50}	5.6 mg/L	(7914)
FISHES: fathead minnow	96h LC_{50}	1.5 mg/L	(2627)
MAMMALS:			
rat, mouse	oral LD_{50}	180-750 mg/kg	(9710, 9836)

(9706)

(9682)

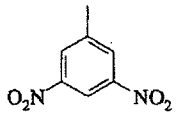
(9621)

(9621)

(1900)

(1901)

3,5-dinitrotoluene (1-methyl-3,5-dinitrobenzene; 3,5-DNT)



(2627)

(7914)

(2627)

$CH_3C_6H_3(NO_2)_2$

(9709, 9710)

$C_7H_6N_2O_4$

CAS 618-85-9

USE: Cathodic depolariser for magnesium batteries. Chemical intermediate.

A. PROPERTIES: molecular weight 182.14; melting point 93°C; density 1.28 at 111°C; log P_{oct} 2.28 (calculated) .

B. AIR POLLUTION FACTORS

Photochemical reactions: $t_{1/2}$: 87 d, based on reactions with OH°(calculated). (8359)

C. WATER AND SOIL POLLUTION FACTORS:

Manmade sources: constituent of condensate water of TNT manufacturing process.
Mobility in soil: K_{oc}: 414 (calculated)

D. BIOLOGICAL EFFECTS:

CRUSTACEANS: water flea	48h LC_{50}	45 mg/l	(2627)
FISHES: fathead minnow	96h LC_{50}	23 mg/l	(2627)
MAMMALS:			
rat, mouse	oral LD_{50}	215-610 mg/kg bw	(10196)

ılculated).

(8481)

dinocap (karathane; crotothane; Arathane; 2(or 4)-isooctyl-4,6(or 2,6)-dinitrophenyl-2-butenoate; (E)-2-(1-methylheptyl)-4,6-dinitrophenyl 2-butenoate; capryldinitrophenyl-crotonate)

1202 glyphosate

A. PROPERTIES: mw 74.03; mp 98°C; 70–75°C with 1.5 mol H_2O decomposes from 40°C onward into formaldehyde, CO_2, and CO; bp approx. 100°C (50% aqueous solution); d 1.33 at 20°C of 50% aqueous solution; solub. miscible; log P_{oct}<0.

B. AIR POLLUTION FACTORS:

ODOR: acetic acid odor.

C. WATER AND SOIL POLLUTION FACTORS:

BIODEGRADATION

Inoculum	*Method*	*Concentration*	*Duration*	*Elimination results*	
Municipal A.S.		39 mg/L	3 d	99% DOC	
			14 d	98.1% DOC	(6260)

D. BIOLOGICAL EFFECTS:

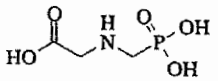
CRUSTACEANS

Daphnia magna Straus	24 h EC_{50}	330 mg/L (50% solution)	(6260)

FISHES

Brachydanio rerio	24 h LC_{50}	194 mg/L (50% solution)	(6260)

glyphosate (*N*-(phosphonomethyl)glycine; glyphosate acid)



$C_3H_8NO_5P$

$HOOCCH_2NHCH_2PO(OH)_2$

CAS 1071-83-6

USES: Herbicide. Organic synthesis.

A. PROPERTIES: colorless crystals; molecular weight 169.08; melting point 189.5°C; vapor pressure < 10^{-7} hPa at 45°C; solubility 10,000 mg/L at 25°C; log P_{oct} 0.001-0.002 (measured).

C. WATER AND SOIL POLLUTION FACTORS:

COD: 0.53 gO_2/g substance = 47% ThOD
ThOD: 1.13 (nitrate and phosphate formation)

Photodegradation: Photodegradation of glyphosate on soil surfaces to aminomethylphosphonic acid (AMPA) is very slow in soil.

Direct photolysis	*$t_{1/2}$ d*	*light source*	*type*	
< 10% after 72 hours		275 watt sun lamp	soil	
19.8% after 31 d	90 d	sun light	soil	
ca 0% after 31 d	413 d	sun light	water	(10302)

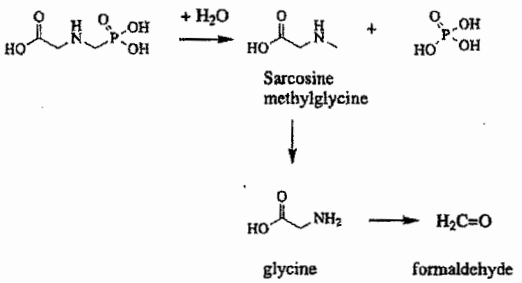
Photolysis: 75% removal from 1% solution in distilled water exposed to sunlight for 2 weeks, but in polluted water only 15% was removed (10296)

Biodegradation

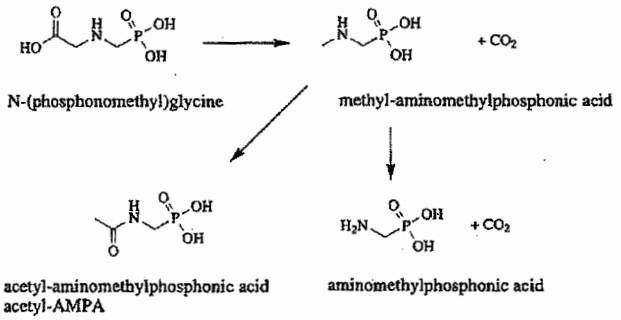
Inoculum	*method*	*concentration*	*duration*	*elimination results*
sediment	EPA Guidelines 1972	5.56 mg/L	45 d	13-29% product

Anaerobic aqueous degradation of glyphosate in the presence of sediment occurs rapidly: $t_{1/2}$ at pH 7 and 25°C: 8.1 d. The primary degradation products are aminomethylphosphonic acid (AMPA) and carbon dioxide. Several low-level unidentified radioloabeled compounds are also produced. However the concentrations of all the unidentified products are below 6.2% of the initial glyphosate concentration. (10302)

Biodegradation: $t_{1/2}$ for degradation in soil approx. 60 d (9600)



Degraded by several *Rhizobiaceae* species, *Pseudomonas* and *Arthrobacter atrocyoneus* when utilised as sole phosphorus source. Sarcosine was the immediate degradation product indicating that the initial cleavage of glyphosate was at the C-P bond, followed by oxidation of sarcosine to glycine and formaldehyde (10291; 10292; 10293; 10294)



Glyphosphate is metabolized by two species of *Ochrobactrum anthropi*. Both species metabolize glyphosate via the aminomethylphosphonate (AMPA) pathway. The formation of N-methyl AMPA is common to both species but the formation of N-acetyl AMPA is only observed in one of the species. (10295)

In laboratory tests:

Kickapoo sandy loam at 4 mg/kg and 25°C:	DT_{50}: 1.9 d
	DT_{90}: 8.1 d
Dupo silt loam at 4 mg/kg and 25°C:	DT_{50}: 2.1 d
	DT_{90}: 10.8 d (10302)

Dissipation half lives: Glyphosate was applied at the maximum annual rate of 8.9 a.e./ha to 8 separate bare ground test plots in different states of the USA: glyphosate: $t_{1/2}$: median: 14.9 d; range: 1.7-142 d metabolite AMPA: $t_{1/2}$: median: 240 d; range 131-958 d (10302)

Soil leaching tests: Result of all studies demonstrate that glyphosate is strongly absorbed to soils and has limited potential to leach through soil or move off-site due to surface run-off. (10302)

Impact on biodegradation:

Degradation of cellulose, starch, protein amd leaf litter was not affected at a level of glyphosate of 25 mg/kg dry soil. Glyphosate did not affect nitrogen fixation at this level over a period of 84 d. (10152)

Waste water treatment

Effectively removed from river water by coagulation and filtration. Removal by activated carbon was less efficient from river water than from distilled water (10297)

1204 glyphosate

Soil sorption:	Lintonia fine sand:	K_d: 22-15	
	Cattail swamp sediment:	K_d: 175-205	(10302)
	clay and clay soils	K_{oc}: 8-138	(10298)

Degradation: Degradation in soil is microbial. After 16 weeks, <3% of the starting material is detectable. Degradation products are carbon dioxide, water, nitrate, and phosphate. (2962)

D. BIOLOGICAL EFFECTS:

Bioaccumulation	*concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Crustaceans					
Procambarus simulans	3000	28 d	9	edible portions	
			8	total body	(10302)
Molluscs					
Rangia cuneata	500	35 d	9.6	edible portions	
	3000	28 d	4.8	edible portions	(10302)
Fishes					
Ictalurus punctatus	< 10,000	14 d	0.18	total body	
	1,000	10 d	0.26	total body	
Micropterus salmoides	< 10,000	14 d	0.04	total body	
	< 10,000	14 d	0.03	total body	(10302)

BACTERIA:

Biotox™ test	*Photobacterium phosphoreum*	5min EC_{20}	0.75 mg/L	
		5min EC_{50}	2.2 mg/L	
Microtox™ test	*Photobacterium phosphoreum*	5min EC_{50}	7.7 mg/L	(7023)
Soil bateria		84d NOEC	>25 mg/kg	(7023)

ALGAE:

Selenastrum capricornutum in algal assay medium

inhib. of oxygen evolution	EC_{50}	0.01 mg/L	
growth inhib.	EC_{50}	0.0038 mg/L	
photosynthesis inhib.	EC_{50}	35 mg/L; 44 mg/L; 70 mg/L	
nitrogen fixation inhib.	EC_{50}	<25 mg/L; <100 mg/L	(2624)
	72h EC_{50}	1.1 mg/L	
	72h EC_{100}	3.2 mg/L	(7024)
inhib.of oxygen evolution	EC_{50}	0.01 mg/L	
growth inhib.	EC_{50}	0.0038 mg/L	
photosynthesis inhib.	EC_{50}	35; 44; 70 mg/L	
nitrogen fixation inhib.	EC_{50}	< 25; < 100 mg/L	(2624)
Anabaena flos-aquae growth inhibition	7d EC_{50}	15 mg/L	
Naviculla peliculosa growth inhibition	7d EC_{50}	42 mg/L	
Selenatsrum capricornutum growth inhibition	7d EC_{50}	13.8; 485 mg/L	
	7d NOEC	45 mg/L	
Skeletonema costatum growth inhibition	7d EC_{50}	0.64 mg/L	
	96h EC_{50}	1.3 mg/L	
Lemna gibba growth inhibition	14d EC_{50}	25.5 mg/L	
	14d NOEC	16.6 mg/L	(10302)

INSECTS:

Anopheles quadrimaculatus	24h LC_{50}	673 mg/L	
Chirinomus riparius midge larvae	48h EC_{50}	5,600 mg/L	(10290)
Procambarus clarki	4d LC_{50}	47 mg/L	(2625)

CRUSTACEANS:

Daphnia pulex	48h LC_{50}	42 µg/L	(2127)
Korean shrimp *(Palaemon macrodactylus)*	96h LC_{50},S	14 (8.2–26) ppb	(2353)
sand shrimp *(Crangon septemspinosa)*	96h LC_{50},S	8 ppb	(2327)
grass shrimp *(Palaemonetes vulgaris)*	96h LC_{50},S	440 ppb	(2327)
hermit crab *(Pagurus longicarpus)*	96h LC_{50},S	55 ppb	(2327)
isopod *(Asellus)*	24h LC_{50}	100 ppb	(1681)
pelecypod *(Crassostrea virginica)*	96h EC_{50}-F	1.5 mg/L	
decapod *(Penaeus duorarum)*	96h EC_{50}-F	0.11 mg/L	
decapod *(Palaemonetes vulgaris)*	96h EC_{50}-F	1.06 mg/L	(1138)
FISHES:			
Pimephales promelas	96h LC_{50}	56 µg/L	(2113)
Lepomis macrochirus	96h LC_{50}	19 µg/L	(2113)
Lepomis microlophus	96h LC_{50}	17 µg/L	(2107)
Salmo gairdneri	96h LC_{50}	19 µg/L	(2119)
Oncorhynchus kisutch	96h LC_{50}	59 µg/L	(2119)
Oncorhynchus tschawytscha	96h LC_{50}	17 µg/L	(2189)
mummichog *(Fundulus heteroclitus)*	96h LC_{50}	50 ppb	(2328)
striped killifish *(Fundulus majalis)*	96h LC_{50},S	32 ppb	(2329)
Atlantic silverside *(Menidia menidia)*	96h LC_{50},S	3 ppb	(2329)
striped mullet *(Mugil cephalus)*	96h LC_{50},S	194 ppb	(2329)
American eel *(Anguilla rostrata)*	96h LC_{50},S	10 ppb	(2329)
bluehead *(Thalassoma bifasciatum)*	96h LC_{50},S	8 ppb	(2329)
bluegill:	96h LC_{50}	0.190 ppm	
rainbow trout	96h LC_{50}	0.150 ppm	(1878)
northern puffer *(Sphaeroides maculatus)*	96h LC_{50},S	188 ppb	(2329)
threespine stickleback *(Gasterosteus aculeatus)*	96h LC_{50},S	112 ppb	(2333)
Cyprinodon variegatus	96h LC_{50},FT	3.68 µg/L	
Lagodon rhomboides	96h LC_{50},FT	3.77 µg/L	
Leiostomus xanthurus	96h LC_{50},FT	0.85 µg/L	(1138)
minnow	24h LC_{50}	13 ppb	(1681)
fathead minnow	LC_{50},F	7.02 µg/L at 25°C	
	MATC	0.86 µg/L	(443)
Pagurus longicarpus	96h LC_{50}	55 µg/L	(1575)
Cyprinodon variegatus	96h LC_{50}	3.7–10.5 µg/L	
	MATC, early life stage	1.58 µg/L	
	MATC life cycle	1.4 µg/L	(2643)

Biotransfer factor in beef: log B_b: –1.81
Biotransfer factor in milk: log B_m: –2.49
Bioconcentration factor for vegetation: log BCF_v: –1.48 (2644)

heptachlorepoxide (Velsicol 53-CS-17; ENT 25,584; 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methanoindene)

$C_{10}H_5Cl_7O$

CAS 1024-57-3

ORIGIN: degradation product of heptachlor.

A. PROPERTIES: molecular weight 389.30; melting point 160-161.5°C; vapor pressure 2.6 x 10_{-6} mmHg at 20°C; solubility ca. 0.3 mg/L at 25°C; log P_{oct} 5.4.

B. AIR POLLUTION FACTORS:

(2127) *Incinerability:* thermal stability ranking of hazardous organic compounds: rank 193 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

(2353)
(2327)

C. WATER POLLUTION FACTORS:

(2327) *Aquatic reactions:*

(2327) persistence in river water in a sealed glass jar under sunlight and artificial fluorescent light—initial conc. 10 µg/L: after 8 weeks 100% of original compound still found. (1309)

(1681) Volatilisation from model river water: $t_{1/2}$: 60 h . (8383)

(1138) dimensionless distribution coefficient at initial conc. = 1 mg/L:
on mixed liquor: 17,900 (2395)

(2113) Biodegradation:
(2113) Degraded to 1-exohydroxychlordene by soil microflora at 28°C:
(2107) conversion rates 2.8% after 4 weeks
(2119) 5.8% after 8 weeks
(2119) 12% after 12 weeks (10303)
(2189) Degradation in thick digester sludge under aerobic conditions at 35°C: $t_{1/2}$: 25 d. At 20°C under aerobic or anaerobic conditions in 60 d: no significant degradation. (7056)
(2328)
(2329) Mobility in soils:
(2329) Certamite clay: K_{oc}: 100
(2329) river water suspended solids: K_{oc}: 10,000-20,000 (7056; 10304)
(2329)
(2329)

D. BIOLOGICAL EFFECTS:

(1878) *Residues:*

(2329) goby fish *(Acanthogobius flavimanus)* collected at the seashore of Keihinjima along Tokyo Bay—Aug. 1978: residue level: 1 ppb (1721)

(2333) residues in Canadian human milk: 1967: avg.: 3 ng/g whole milk
1970: avg.: 4 ng/g whole milk
1975: avg.: 1 ng/g whole milk (1376)

(1138) ringed seal, Greenland, fat: 0.026 mg/g (1180)
(1681)

(443) *Bioaccumulation:*
(1575) pelecypod *(Mytilus edulis)*: exposure: 0.22–1.9 µg/L, 50h:
bioaccumulation factor: BCF: 1,700 (1477)
log BAF: rainbow trout Lake Ontario (U.S.A.): 5.55 l/kg(lp) (2442)
log BCF: fathead minnow: 4.16 (2606)

(2643) MUSSEL: *Mytilus edulis* BCF: 1,700 (2617)

Toxicity:

(2644)

decapod *(Penaeus duorarum)*:	96h LC_{50},F	0.04 µg/L	(1138)
biotransfer factor in beef	log B_b:	−1.10	
biotransfer factor in milk	log B_m:	−1.45	
bioconcentration factor for vegetation	log BCF_v:	−1.62	(2644)

BACTERIA:

Photobacterium phosphoreum Microtox test	5min EC_{50}	25 mg/L	(8899)

MAMMALS:

rat, mouse	oral LD_{50}	39-62 mg/kg bw	(10305; 10306)

1,4,5,6,7,8,8-heptachlor-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methanoindene *see* heptachlorepoxide

ı,4,7,7a-tetrahydro-4,7-

.6 mmHg at 20°C; solubility

BIODEGRADATION

Inoculum	*Method*	*Concentration*	*Duration*	*Elimination results*	
	Sapromat test			>60% ThOD	(6205)
	Zahn-Wellens test			>70% DOC	(6205)

C. BIOLOGICAL EFFECTS:

BACTERIA:

Adapted A.S.	30 min EC_{10}	>1,000 mg/L	(6205)
Pseudomonas putida	17 h EC_{10}	6,260 mg/L	
(cell multiplication inhibition test)	17 h EC_{50}	9,010 mg/L	
	17 h EC_{90}	>10,000 mg/L	(6203)

ALGAE:

Scenedesmus subspicatus	96 h EC_{20}	300 mg/L*	
(cell multiplication inhibition test)	96 h EC_{50}	>500 mg/L	
	96 h EC_{90}	>500 mg/L	(6204)

CRUSTACEANS

Daphnia magna Straus	24– 48 h EC_0	500 mg/L	
	24– 48 h EC_{50}	>500 mg/L	
	24– 48 h EC_{100}	>500 mg/L	(6203)

FISHES:

Leuciscus idus	96 h LC_{50}	2,200– 4,600 mg/L	(6202)

1-methyl-4-*tert*-butylbenzene *see p-tert*-butyltoluene

methyl-tert-butylether (2-methoxy-2-methylpropane; MTBE; tert-butyl methyl ether; methyl 1,1-dimethylethyl ether; MTBE; 2-oxa-3,3-dimethylbutane)

$C_5H_{12}O$

$CH_3OC(CH_3)_3$

CAS 1634-04-4

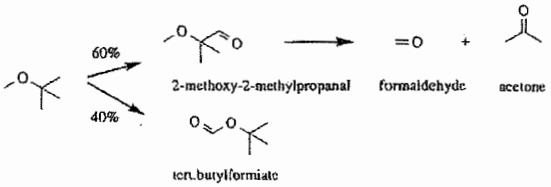
USES: Octane improver in motor gasoline as a substitute for lead alkyls. Catalyst. Solvent for cholesterol gallstones. Chromatographic eluent.

A. PROPERTIES: mw 88.1; mp – 108°C; bp 55.3°C; vp 268 hPa at 20°C; d 0.74 at 20°C; solub. 10,000 mg/L at 10°C, 50,000 mg/L at 25°C; log P_{oct} 1.1 (measured).

B. AIR POLLUTION FACTORS:

Photochemical reactions: $t_{1/2}$: 2.5-2.8; 3.5; 5– 6 d, based on reactions with OH°(calculated). (7535, 7536, 7537, 7538)

PHOTOCHEMICAL OXIDATION:

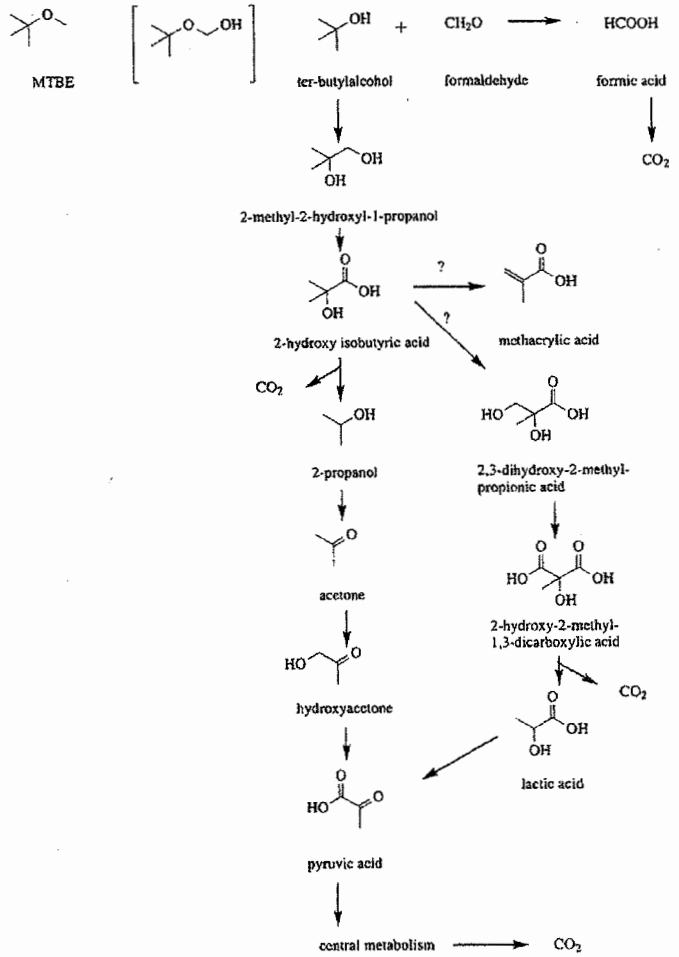


(7539)

C. WATER AND SOIL POLLUTION FACTORS:

Volatilization from water at 25°C
from model river: $t_{1/2}$: 4.1 h
from model pond: $t_{1/2}$: 2 d (7, 8)

BIODEGRADATION PATHWAYS



Proposed biochemical pathway for biodegradation of MTBE

BIODEGRADATION

Inoculum	*Method*	*Concentration*	*Duration*	*Elimination results*	
Municipal A.S.	Closed bottle test	2 mg/L	28 d	0% ThOD	(7533)
Mixed	Modified closed bottle test	2 mg/L	28 d	5.4% ThOD*	
A.S.			21 d	1% ThOD	(4)

*After 14 d acclimation period at 5 mg/L (7534)
K_{oc}: 11 (calculated) (8902)

CAS 64741-65-7

USES AND FORMULATIONS: a complex combination of hydrocarbons produced by distillation of the reaction products of isobutane with monoolefinic hydrocarbons usually ranging in carbon numbers of C_3 to C_5. It consists of predominantly branched chain saturated hydrocarbons having carbon numbers predominantly in the range of C_9 through C_{12} and boiling in the range of approx. 180 to 220°C. Used as a solvent in the cosmetic industry, in paints and for the treatment of surfaces. (8958)

A. PROPERTIES: melting point <-70°C; boiling point 184-217°C; vapor pressure 1.1 hPa at 20°C, 6.1 hPa at 50°C; solubility 10 mg/L at 20°C; log P_{oct} >6.7, <7.2.

B. AIR POLLUTION FACTORS:

Photochemical reactions: $t_{1/2}$: <30 d, based on reactions with OH°(calculated). (8288)

C. WATER AND SOIL POLLUTION FACTORS

ThOD 3.4 gO_2/g product (8959)

Biodegradation (8956)

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
	Closed Bottle Test		5 days	2-3% ThOD	
			28 days	15-22% ThOD	(8287)
	Modified Sturm Test		28 days	2-12% ThCO2	(8287)

D. BIOLOGICAL EFFECTS:

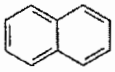
ALGAE:			
Scenedesmus subspicatus (cell multiplication)	72h EC_{50}	>1000 mg/L	(8287)
CRUSTACEANS:			
Daphnia magna	24h EC_{50}	>1000 mg/L	(8287)
FISHES:			
Oncorhynchus mykiss	96h LC_{50}	>1000 mg/L	(8287)

naphtha, heavy aromatic

D. BIOLOGICAL EFFECTS:

CRUSTACEANS:			
Daphnia magna	48h LC_{50}	0.42–2.3 mg/L	(1927)
FISHES:			
fathead minnow	96h LC_{50}	4.2–21 mg/L	
bluegill	96h LC_{50}	2.1–4.2 mg/L	(1927)

naphthalene (tar camphor)



$C_{10}H_8$

CAS 91-20-3

MANUFACTURING SOURCE: petroleum refining; coal tar distillation.

USERS AND FORMULATION: moth ball mfg.; mfg. alpha and beta naphthols and pesticides, fungicides, dyes, detergents and wetting agents, phthalic anhydride, synthetic resins, celluloids, lampblack, smokeless powder; solvent; lubricants; motor

fuel mfg.; cutting fluid, synthetic tanning, preservative; emulsion breaker; asphalt and naphtha constituent, petroleum, coal tar.

in commercial coal tar	150 mg/kg	
constituent of coal tar creosote	11 wt %	
constituent of diesel fuel	350–1,500 mg/L	
in aqueous phase of diesel fuel	0.08–0.3 mg/L	
constituent of coals	0.34–0.65 mg/kg	
in soluble fraction of leachates	0.04–0.97 μg/L	
in suspended fraction of leachates		<0.02–5.2 mg/kg
in S. Louisiana crude oil	400 mg/L	
in Kuwait crude oil	400 mg/L	
in no. 2 fuel oil	4,000 mg/L	
in bunker C fuel oil	1,000 mg/L	
in natural gas consumer distribution lines in New Mexico, U.S.A.	21–55 μg/m^3	

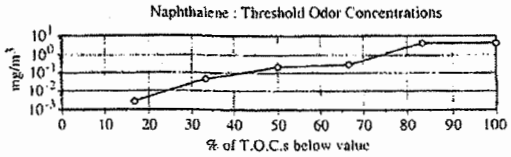
diesel-water partition coefficient: log K_{dw} = 3.68

A. PROPERTIES: white flakes or powder; molecular weight 128.16; melting point 80.2°C; boiling point 217.9°C sublimes; vapor pressure 1 mm at 53°C; vapor density 4.42; d 1.15 solubility 19; 30; 38 mg/L; at 22°C in seawater: 20 ± 2 mg/L; 31–34 mg/L in distilled water at 25°C; THC 1,231 kcal/mole; LHC 1,208 kcal/mole; log P_{oct} 3.01; 3.32; 3.45.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.191 ppm, 1 ppm = 5.24 mg/m^3.

Manmade sources:
- in coal tar pitch fumes: 0.9 wt % (516)
- in emissions from open burning of scrap rubber tires: 486–816 mg/kg of tire (2950)

Odor:



(57, 307, 610, 684, 753, 755)

O.I. at 20°C = 2,400 (316)

Indoor/outdoor glc's winter 1981/1982 and 1982/1983, the Netherlands:

	μg/m^3 median	maximum	
pre-war homes	<0.3	4	
post-war homes	<0.3	14	
homes <6 years old	<0.3	7	
outdoor	<0.3	<0.3	(2668)

Inside and outside 15 living rooms in Northern Italy (1983–1984):

4–7 d averages	lowest	mean	highest value (all in μg/m^3)	
indoor	<1	11	70	
outdoor	<1	2	11	(2756)

Incinerability:
Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 107°C.
Thermal stability ranking of hazardous organic compounds: rank 5 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

C. WATER AND SOIL POLLUTION FACTORS:

Oxidation parameters:

BOD_5:	0% of ThOD	(274, 41, 27, 275, 220)
BOD_{25}:	64% ThOD in seawater/inoculum: enrichment cultures of hydrocarbon-oxidizing bacteria	(521)
COD:	80% ThOD (0.05 *n* Cr_2O_7)	(274)
	22% ThOD	(220)
ThOD:	2.99	(274)

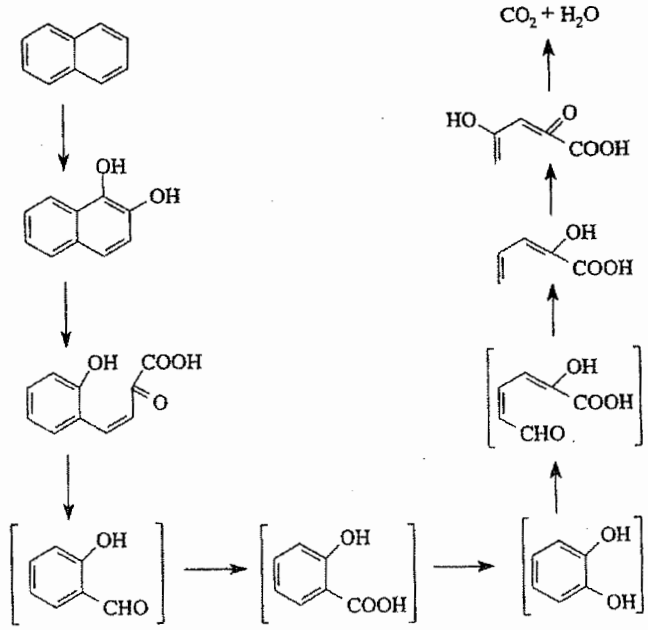
Reduction of amenities: approx. conc. causing adverse taste in FISH:

Rudd	1.0 mg/L	(41)
tainting of fish flesh	1.0 mg/L	(81)
T.O.C. in water	0.5 mg/L	(296)
	0.005 mg/L	(295)
	0.0068 mg/L	(279, 403)
	0.001 mg/L	(301)
	0.068 ppm	(326)

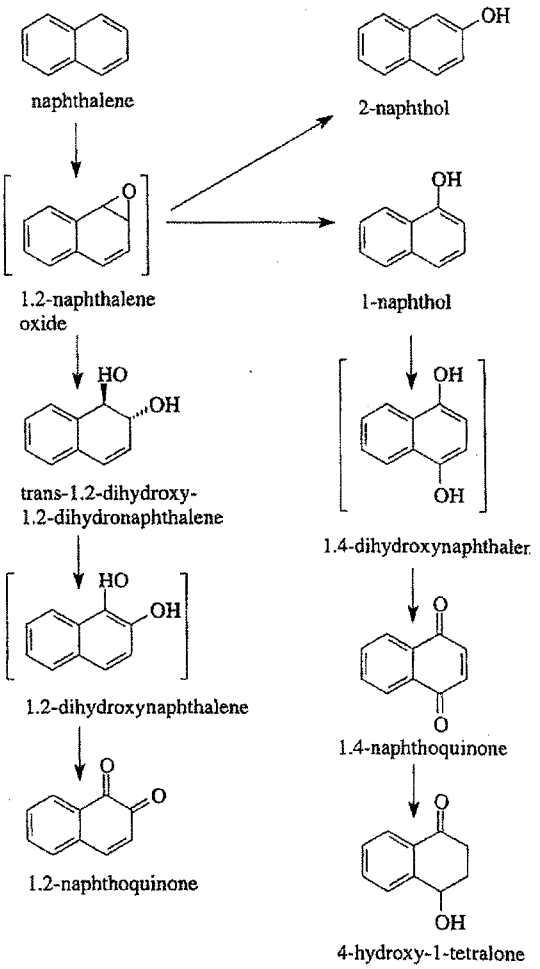
Biodegradation: biodegradation to CO_2:

sampling site	*conc., µg/L*	*month*	*incubation time, h*	*degradation rate, µg/L/d ×10³*	*turnover time, d*		
control station	30	—	—	730 ± 70	41		
near oil storage tanks	30	—	—	2,800 ± 300	11		
near oil storage tanks	60	—	—	4,700 ± 100	13		
near oil storage tanks	30	—	—	840 ± 90	36		
Skidaway River	30	Jan.	24	70 ± 8	430		
Skidaway River	30	May	24	820 ± 110	37		
Skidaway River	15	Aug.	24	420 ± 80	36		
Skidaway River	30	Aug.	24	680 ± 90	45		
Skidaway River	60	Aug.	24	1,200 ± 70	60		
estuarine	30	—	—	870 ± 20	34		
coastal	30	—	—	330 ± 40	230		
Gulf Stream	30	—	—	12 ± 7		2,500	(381)

Microbial degradation to CO_2—in seawater at 12°C—in the dark after 24 hour incubation at 50 µg/L: degradation rate: 0.10 µg/L/d—turnover time 500 d; after addition of aqueous extract of fuel oil 2: degradation rate: 1.0–5.0 µg/L/d—turnover time: 10–22 d. (4077)



Metabolic pathway for the degradation of naphthalene by certain *Pseudomonas* species (1049)



Proposed sequence for the metabolism of naphthalene by *Cunninghamella elegans* (1219)
in leachate from test panels freshly coated with coal tar:
influent: 0.004 µg/l
effluent: 0.025 µg/l (1874)
60 ml/min pure water that was passed through 25 ft, 1/2 in. I.D. tube of general chemical grade P.V.C. (430)
contained 1.7 ppb naphthalene, which constituted 16% of total contaminant concentration.
Göteborg (Sweden) sew. works 1989–1991: infl.: 0.1–15 µg/l; effl.: n.d. (2787)

Aquatic reactions: evaporation:

Calculated half-life in water at 25°C and 1 m depth, based on evaporation rate of 0.096 m/hr: 7 hr. (437)
Adsorption: in estuarine waters: at 30 µg/l, 0.7% is adsorbed on particles after 3 hours. (381)

Water quality:
- in Delaware River (U.S.A.): conc. range: winter: 0.7–0.9 ppb (1051)
- in Zürich Lake; at surface: 8 ppt; at 30-m depth: 52 ppt
- in Zürich tap water: 8 ppt (513)
- in Eastern Ontario drinking waters (June–Oct. 1978): 0.6–7.5 ng/l (n = 12)
- in Eastern Ontario raw waters (June–Oct. 1978): 2.4–3.3 ng/l (n = 2) (1698)

Waste water treatment:

(1049) ion exchange: adsorption on Amberlite XAD-2: 100% retention at 0.05 mg/l influent conc. (40)
compounds identified from the oxidation with chlorine dioxide:
monochloronaphthalene; 1,4-dichloronaphthalene; phthalic acid (1696)

Soil quality: typical values in Welsh surface soil (U.K.), average of 20–5 cm cores:

mean: 8.7 µg/kg dry wt
range: <1.0–131 µg/kg dry wt (2420)

Soil sorption:

K_{oc}:	for Fullerton soil, 0.06% organic carbon:	960	
	for Apison soil, 0.11% organic carbon:	1,000	
	for Dormont soil, 1.2% organic carbon:	400	(2599)

Degradation in soil: bioremediation of diesel-contaminated soil: 0-time conc., 8.3 mg/kg of soil:

% remaining	*without bioremediation*	*with bioremediation*	
after 2 weeks:	5%	2.6%	
after 12 weeks	<1%	<1%	(2384)

Degradation in soil system at initial conc. of 7 mg/kg soil: $t_{1/2}$: 0.1; 125 days. (2903)

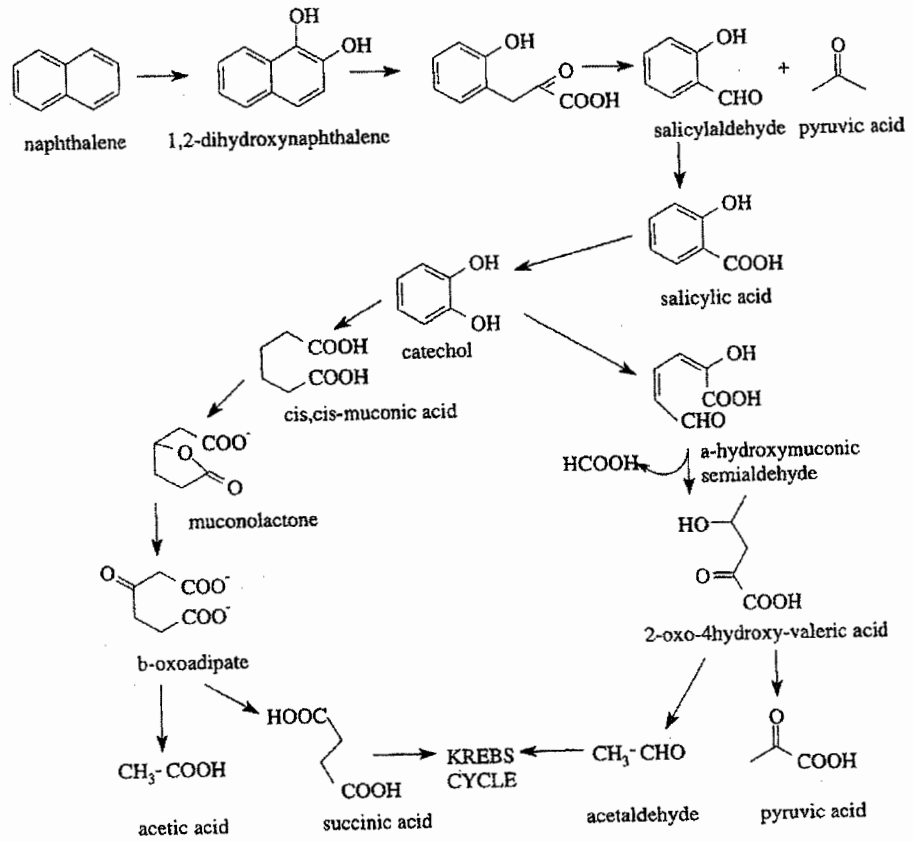
Biodegradation half-lives in non-adapted aerobic subsoil:

groundwater Texas: 2 days
groundwater Florida: 7 days
(1219) sand Texas: >485 days
sand Oklahoma: 3,000 days (2695)
(1874) Aerobic slurry bioremediation reactor with mixed aeration chamber, treating a petrochemical waste sludge at 3.5 to 7.5% solids containing approx. 25% oil and grease and 0.5 to 2.5 grams of waste material per gram of microorganisms, at 22–24°C during batch treatment:
(430) mixed liquor: infl.: 9.2 mg/l; effl. after 15 days: <2.5 mg/l
(2787) waste residues: infl.: 56 mg/kg; effl. after 90 days: <2.5 mg/kg (2800)

Initial oxidation products of soil microorganisms:

(437)
(381)

(1051)	*Cunninghamella elegans*	*trans*-naphthalene diol
		4-hydroxy-1-tetralone
		1,2-naphthoquinone
(513)		1,4-naphthoquinone
		1-naphthol
(1698)		2-naphthol
	Saccharomyces cerevisiae	*trans*-naphthalene diol
		1-naphthol
		2-naphthol (2905)



Sampling and analysis:

recovery with open-pore polyurethane (OH/NCO = 2.2): 56–98%, depending upon load- (29)
quantitative elution with methanol
extraction efficiency of macro-reticular resins: sample flow: 20 ml/min; pH 5.7; conc.

10 ppm:	X AD-2: 90% X AD-7: 93%	(370)

D. BIOLOGICAL EFFECTS:

Bioaccumulation: uptake and depuration by oysters (*Crassostrea virginica*) from oil-treated enclosure:

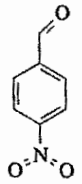
time of exposure, days	depuration time, days	concentration oyster, µg/g	water, µg/l	BCF oyster/water
2	—	30	5	6,000
8	—	12	3	4,000
2	7	1	—	—
8	7	2	—	—
8	23	<0.5	—	—

$t_{1/2}$ for depuration: 2 days (957)

Oysters: uptake and release:

exposure period, days	conc. in oyster*, µg/g	conc. in water, µg/l	dep. time, days	conc. oyster, µg/g	conc. water, µg/l
2	8.6 (4.6)	27	14	0.1	0

1612 4-nitrobenzamide



$C_7H_5NO_3$

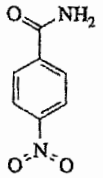
CAS 55-16-8

A. PROPERTIES: molecular weight 151.12.

D. BIOLOGICAL EFFECTS:

Toxicity to microorganisms: nitrification inhib. EC_{50}: 87 mg/L. (2624)

4-nitrobenzamide



$O_2NC_6H_4CONH_2$

$C_7H_6N_2O_3$

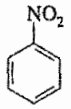
CAS 619-80-7

A. PROPERTIES: molecular weight 166.14; melting point 200-201°C; solubility 160 mg/L; log P_{oct} 0.82.

D. BIOLOGICAL EFFECTS:

ALGAE:			
Tetrahymena pyriformis	48 IC_{50}	100 mg/L	(2704)
FISHES:			
Pimephales promelas	30-35d LC_{50},F	132 mg/L	(2704)
Pimephales promelas	96h LC_{50}	133 mg/L	(2709)

nitrobenzene (oil of mirbane)



$C_6H_5NO_2$

$C_6H_5NO_2$

CAS 98-95-3

MANUFACTURING SOURCE: organic chemical industry.

USERS AND FORMULATION: mfg. aniline and dyestuffs; solvent recovery plants; mfg. rubber chemicals, drugs, photographic chemicals; refining lubricants oils; solvent in TNT production; solvent for cellulose ethers; cellulose acetate mfg.; constituent in metal polish and shoe polish formulations.

A. PROPERTIES: yellow liquid; molecular weight 123.1; melting point 6°C; boiling point 211°C; vapor pressure 0.15 mm at 20°C, 0.35 mm at 30°C; vapor density 4.25; d 1.20 at 25/4°C; solubility 1,900 mg/L at 20°C, 8,000 mg/L at 80°C; THC 739 kcal/mole; LHC 727 kcal/mole; sat. conc.: 1.0 g/m^3 at 20°C, 2.3 g/m^3 at 30°C; log P_{oct} 1.85; 1.88; 2.45; 2.93.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.20 ppm, 1 ppm = 5.12 mg/m^3.

Odor: characteristic quality: shoe polish, bitter almonds.
(21, 57, 291, 306, 602, 604, 606, 610, 678, 682, 704, 710, 741, 793, 871)

(2624)

human odor perception	0.0182 mg/m^3	
human reflex response: no response	0.008 mg/m^3	
adverse response	0.0129 mg/m^3	
animal chronic exposure: no effect	0.008 mg/m^3	
adverse effect	0.008 mg/m^3	(170)
O.I. at 20°C = 200		(316)

Incinerability:
Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 655°C.
Thermal stability ranking of hazardous organic compounds: rank 142 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

C. WATER AND SOIL POLLUTION FACTORS:

BOD_5:	0% ThOD at <440 mg/L	(41, 27)
ThOD:	1.5; 1.95	(27)

).82.

Manmade sources: Göteborg (Sweden) sewage works 1988-1991: influent: n.d.-0.5 µg/L; effluent: n.d. (2787)
In Canadian municipal sludges and sludge compost: September 1993-February 1994: mean values of 11 sludges ranged from ND to 5.2 mg/kg dw.; mean: 0.7 mg/kg dw;mean value of sludge compost: ND. (7000)

100 mg/L (2704)

Reduction of amenities: faint odor at 0.03 mg/L: (129)

132 mg/L (2704)
133 mg/L (2709)

odor threshold conc. (detection): 0.2 mg/kg (894)
in river Maas (Netherlands): average in 1973: n.d. to 0.07 µg/L (342)

Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
domestic sewage	Closed Bottle Test		5 d	<1% ThOD	(9118)
domestic sewage	Closed Bottle Test	3 mg/L	30 d	>90% ThOD	(9109)
A.S. industrial	Zahn-Wellens Test*		1 d	26% DOC	
			4 d	63% DOC	
			7 d	91% DOC	
			10 d	86% DOC	
no inoculum	Zahn-Wellens Test*		1 d	34% DOC	
			3 d	54% DOC	
			7 d	72% DOC	
			10 d	79% DOC	(9110)

A.S. municipal	Manometric respirometry	60 mg/L	1 d	0% ThOD	
			25 d	0% ThOD	
			27 d	10% ThOD	
			35 d	52% ThOD	(9111)
municipal effluent filtered	Modified OECD Screening Test*		1 d	9% DOC	
			7 d	65% DOC	
			14 d	96% DOC	
no inoculum	Modified OECD Screening Test*		1 d	12% DOC	
			7 d	58% DOC	
			14 d	88% DOC	
			21 d	88% DOC	(9112)
A.S. industrial	Manometric respirometry	70 mg/L	8 d	57% ThOD	(9113)
		180 mg/L	12 d	50% ThOD	(9114)
A.S. industrial adapted	Modified OECD Screening Test	3-10 mg/L		100% product	(9115)
different suldges	Modified MITI test	100 mg/L	14 d	3.3% ThOD	(9116)

* with or without inoculum the same reduction of DOC is obtained indicating that biodegradation did not occur in this test.

Adapted A.S. at 20°C—product is sole carbon source: 98% COD removal at 14 mg COD/g dry inoculum/h. (327)

Disappearance in soil at 100 mg/kg and 20°C under aerobic laboratory conditions: $t_{1/2}$: 9.1 d; confidence limits: 6.7–14.1 d. (2366)

Degradation $t_{1/2}$: 625 d in activated sludge. (2368)

Waste water treatment:

A.C.: adsorbability: 0.196 g/g carbon; 96% reduction at influent conc. 1,023 mg/L (32)

Air stripping constant: $k = 0.84\ d^{-1}$ at influent conc. 250 mg/L (82)

Soil sorption: K_{oc}: 30–103 at 1.0 mg/L. (2588)

Impact on biodegradation processes:

inhibition of degradation of glucose by *Pseudomonas fluorescens* at 30 mg/L
inhibition of degradation of glucose by *E. coli* at 600 mg/L (293)
act. sludge respiration inhib. EC_{50}: >100 mg/L
OECD 209 closed system inhib. EC_{50}: >100 mg/L (2624)

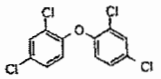
D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Fishes: *Cyprinus carpio*	12	42 d	1.6-7.7	total body	
	125	42 d	3.1-4.8	total body	(9116)
fathead minnow			15		(2606)
Algae: *Chlorella fusca*			24	wet weight	(2659)

BACTERIA:

E. coli	LD_0	600 mg/L	(30)
A.S. respiration inhibition	30 min EC_{50}	320 mg/L	(9109)
	3h EC_{50}	100 mg/L	(9121)
	5d EC_{50}	630 mg/L	(9125)
Aerobic heterotrophs	49h IC_{50}	370 mg/L	(9124)
Pseudomonas putida	16h EC_0	34 mg/L	(9109)
	16h EC_3	7 mg/L	(1900)

1946 1,1,2,2-tetrachloroethane



$Cl_2C_6H_3OC_6H_3Cl_2$

$C_{12}H_6Cl_4O$

CAS 42279-28-7

A. PROPERTIES: molecular weight 307.98; log P_{oct} 6.72.

D. BIOLOGICAL EFFECTS:

FISHES: rainbow trout *(Salmo gairdneri)*: BCF 12,400 ± 2,290 (193)

→ **1,1,2,2-tetrachloroethane** (acetylenetetrachloride; Acetosan; Bonaform; Cellon; 1,1-dichloro-2,2-dichloroethane; sym-tetrachloroethane; Westron)

$CHCl_2CHCl_2$

$C_2H_2Cl_4$

CAS 79-34-5

MANUFACTURING SOURCE: Organic chemical industry. (347)

USES AND FORMULATION: mfg. 1,1-dichloroethylene; solvent for chlorinated rubber and other organic materials; insecticide mfg.; bleach mfg.; paint, varnish, rust remover mfg.; soil fumigant; cleansing and degreasing metals; photo films, resins and waxes; extractant of oils and fats; organic synthesis, herbicide; alcohol denaturant. (347)

A. PROPERTIES: Colorless liquid; molecular weight 167.86; melting point –42.5/43.8°C; boiling point 146.4°C; vapor pressure 5 mm at 20°C, 8.5 mm at 30°C; vapor density 5.79; d 1.60 at 20/4°C; solubility 2,900 mg/L at 20°C; saturation concentration in air 46 g/m^3 at 20°C, 75 g/m^3 at 30°C; log P_{oct} 2.39; log H –1.73 at 25°C.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.14 ppm, 1 ppm = 6.98 mg/m^3.

Odor threshold conc.:	<3 ppm	(211)
	20 mg/m^3	(740)
	detection: 50 mg/m^3	(643)

Incinerability:
Temperature for 99% destruction at 2.0-s residence time under oxygen-starved reaction conditions: 690°C.
Thermal stability ranking of hazardous organic compounds: rank 121 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

Tropospheric lifetime (estd.): 0.09 yr.
Ozone depletion potential (estd.): <0.001 per molecule. (2446)
In 4 municipal landfill gases in S. Finland (1989–1990): avg <0.4–0.7, max 1.0 mg/m^3. (2605)

C. WATER AND SOIL POLLUTION FACTORS:

Aquatic reactions:
Environmental hydrolysis $t_{1/2}$ at 25°C and pH 7: 47 years. (2434)
Reductive dehalogenation in anoxic sediment with 6% organic carbon: half-life: 6.6 d at 22°C. (2842)
Abiotic transformation: $t_{1/2}$ at 25°C at pH 7: 102 d; TCA is converted quantitatively to 1,1,2-trichloroethylene by a base-promoted second-order elimination reaction. (2641)
Environmental hydrolysis half-life at 25°C and pH 7: 146 d. (2434)
Methanogenic laboratory column reactor at 35°C in the dark and a liquid detention time of 2 d, at influent conc. of 27 µg/L and 0 weeks acclimation: 97% removal at steady state. (2959)

Biodegradation

Inoculum	*Method*	*Concentration*	*Duration*	*Elimination results*	
Unacclimated	Modified shake flask		24 d	41%	
	River bioassay test			19%	(6100)

Water quality: in rivers in UK (1986): 139 samples from 70 river sites yielded 6 positive values (detection limit: 0.1 µg/L): median of positive values: 0.15 µg/L; maximum: 3.3 µg/L (n.s.i.). (2711)

Reduction of amenities:
Odor threshold: 5 mg/L (84)
T.O.C. in water: 0.5 mg/L (326)

Waste water treatment: evaporation from water at 25°C of 1 ppm solution:
50% after 56 min
90% after less than 120 min (313)
Volatilization from water: from model river: $t_{1/2}$: 6.3 h
From model pond: $t_{1/2}$: 3.5 d (8383, 9258)

Mobility in soils: K_{oc}: 79 in a silt loam soil.

D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*Exposure period*	*BCF*	*Organ/tissue*	
FISHES: fathead minnow			8		
Bluegill			8		(2606)
BACTERIA:					
Activated sludge oxygen consumption inhibition		5 d EC_{50}		300 mg/L	(7047)
Photobacterium phosphoreum (Microtox test)		15 min EC_{50}		4 mg/L	(7047)
		30 min EC_{50}		7.9 mg/L	(8899)
Nitrosomonas sp.		25 d IC_{50}		1.4 mg/L	(8433)
Aerobic heterotrophs isolated from A.S.		5 d IC_{50}		130 mg/L	(8433)
Methanogenic bacterial culture		50 d IC_{50}		4.1 mg/L	(8433)
ALGAE:					
Scenedesmus subspicata inhib. of growth		72 h EC_{50}		26 mg/L	(7047)
CRUSTACEANS:					
Daphnia magna		24 h EC_{50}		11 mg/L	(7047)
FISHES:					
Guppy *(Poecilia reticulata):*		7 d LC_{50}		37 mg/L	(1833)
Fathead minnow, American flagfish		48 h LC_{50}		24 mg/L	(7047)
		96 h LC_{50}		16–20 mg/L	(8433, 8891)
MAMMALS:					
Rat		oral LD_{50}		250–800 mg/kg bw	(9801)

1,2,2,2-tetrachloroethane (1,1,1-2-tetrachloroethane)

CH_2ClCCl_3

$C_2H_2Cl_4$

CAS 630-20-6

USE: Solvent.

A. PROPERTIES: molecular weight 167.85; melting point – 70.2°C; boiling point 138°C; vapor pressure 12 mm Hg at 25°C; d 1.60; solub. 1,100 mg/L at 25°C; log P_{oct} 3.2.

B. AIR POLLUTION FACTORS:

Photochemical reactions: $t_{1/2}$: 550 d, based on reactions with OH°(calculated). (8374)

C. WATER AND SOIL POLLUTION FACTORS:

Waste water treatment: evaporation from water at 25°C of 1 ppm solution:
50% after 43 min
90% after more than 120 min (313)
Volatilization from model river water, estimated $t_{1/2}$: 4.2 h (8383)

Hydrolysis: $t_{1/2}$ >50 yr (estimated). (6102)

Mobility in soil: K_{oc}: 99 (experimental). (6103)

D. BIOLOGICAL EFFECTS:

BACTERIA:			
Activated sludge oxygen consumption inhibition	5 d EC_{50}	523 mg/L	(7047)
Photobacterium phosphoreum Microtox test	30 min EC_{50}	2.8 mg/L	(8899)
	15 min EC_{50}	3 mg/L	(7047)
Nitrosomonas sp	25 d IC_{50}	8.7 mg/L	(8433)
Aerobic heterotrophs isolated from A.S.	5 d IC_{50}	230 mg/L	(8433)
Methanogenic bacterial culture	50 d IC_{50}	1.7 mg/L	(8433)
ALGAE:			
Scenedesmus subspicata inhib. of growth	72 h EC_{50}	48 mg/L	(7047)
CRUSTACEANS:			
Daphnia magna	24 h EC_{50}	32 mg/L	(7047)
FISHES:			
Bluegill sunfish	96 h LC_{50}	20 mg/L	(8102)
MAMMALS:			
Rat, mouse	oral LD_{50}	670, 1,500 mg/kg bw, respectively	(6104)

tetrachloroethylene (perchloroethylene; ethylenetetrachloride; tetrachloroethene)

2044 2,3,4-trichloroanisole

$NH_2C_6H_2Cl_3$

$C_6H_4Cl_3N$

CAS 634-93-5

USE: in photographic materials.

A. PROPERTIES: long needles; molecular weight 196.47; melting point 77.5°C; boiling point 262.4°C; log P_{oct} 3.5.

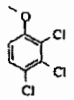
C. WATER POLLUTION FACTORS:

Biodegradation: degradation by *Aerobacter:* 500 mg/L at 30°C
parent: 82% ring disruption in 120 h
mutant: 100% ring disruption in 30 h (152)

D. BIOLOGICAL EFFECTS:

FISHES:			
fathead minnow *(Pimephales promelas):*	96h LC_{50},S	1–10 mg/L	(935)

2,3,4-trichloroanisole (1,2,3-trichloro-4-methoxybenzene)



$C_7H_5Cl_3O$

CAS 54135-80-7

A. PROPERTIES: molecular weight 211.47; melting point 69-71°C; log P_{oct} 4.2.

D. BIOLOGICAL EFFECTS: rainbow trout: laboratory BCF: 1,600–2,300 at 10–66 ng/L. (2399, 2400)

Biouptake by Oligochaete worms Tubifex tubifex *and* Limnodrilus hoffmeisteri: worm/sediment cumulation factor after 79 d at 8°C and 0.61 mg/kg sediment: 0.3; $t_{1/2}$ in worm: could not be determined, concentration increased during the worms' depuration phase! (2618)

ALGAE:			
Minutocellus polymorphus	48h EC_{50}	0.40 mg/L	
Skeletonema costatum	72h EC_{50}	0.63 mg/L	(6159)

→ 1,2,3-trichlorobenzene

$C_6H_3Cl_3$

CAS 87-61-6

MANUFACTURING SOURCE: organic chemical industry, pesticide mfg. (347)

USERS AND FORMULATION: solvent for high-melting products; coolant in electrical installations and glass tempering; mfg. 2,5-dichlorophenol; polyester dyeing; termite preparations, synthetic transformer oil; lubricants; heat-transfer medium, insecticides. (347)

MAN-CAUSED SOURCES (WATER AND AIR): general lab use; agricultural runoff; termite control operations; use of transformer oil. (347)

A. PROPERTIES: plates; molecular weight 181.46; melting point 52°C; boiling point 219°C; vp: 0.0004 atm at 20°C; solubility 12 mg/L at 22°C; log P_{oct} 4.11; 4.20.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.13 ppm, 1 ppm = 7.54 mg/m^3. (57)

Air quality: indoor/outdoor glc's winter 1981–1982 and 1982–1983 the Netherlands:

	μg/m^3 median	μg/m^3 maximum	
pre-war homes	<0.8	3	
post-war homes	<0.8	3	
homes <6 years old	<0.8	28	
outdoors	<0.8	<0.8	(2668)

Manmade sources: in municipal landfill gases in S. Finland (1989–1990): avg <0.01–0.01, max 0.03 mg/m^3. (2605)

C. WATER POLLUTION FACTORS:

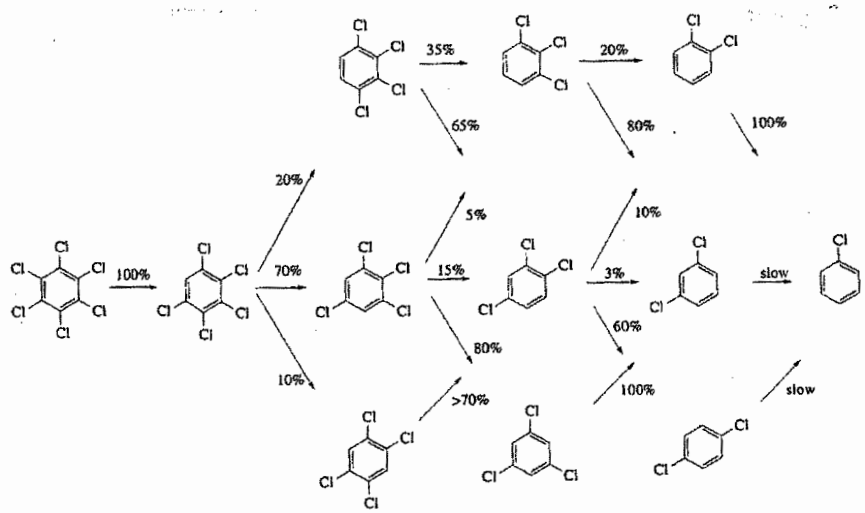
Manmade sources:
anaerob. digest. sew. sludge from municipal area, U.K. 1989: mean: 3.6 μg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area, U.K. 1990: mean: 259 μg/kg (2688)

Occurrence in sewage sludges, NW England 1989:

urban	mean	8 μg/kg dry wt	SD	6.6 μg/kg dry wt	
urban/industrial	mean	246 μg/kg dry wt	SD	236 μg/kg dry wt	(2953)

Reduction of amenities: T.O.C. = 0.01 mg/L. (225)

Biodegradation: degradation by *Pseudomonas:* 200 mg/L at 30°C
parent: 87% ring disruption in 120 h
mutant: 100% ring disruption in 43 h (152)
Degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.07 mg/L: 27% removal in 32 d. Biodegradation may have been the mechanism of removal for part or all of the reductions observed. (2653)
Reductive dechlorination in sediment under sulfate reducing conditions at 25°C: half life period assuming peudo first order kinetics: 23 d. (7041)



Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

Water treatment: water solubility increases to 25 mg/L by addition of surfactants:

surfactant	*surfactant conc., mg/L*	*log* K_{mw}*
Triton X-114	150	3.95
Triton X-100	190	3.82
Brij 35	300	3.31
cetyltrimethylammoniumbromide	300	3.80
sodium dodecyl sulfate	2,300	3.54

* log K_{mw} = micelle-water partition coefficient for trichlorobenzene (2364)

Degradation in soil biodegradation half-lives in nonadapted aerobic subsoil: (n.s.i.); sand Oklahoma: 160, >485 d. (2695)

Water and sediment quality:

in Delaware River (U.S.A.): conc. range:	winter:	0.5–1 µg/L	
(n.s.i.)	summer:	n.d.	(1051)

in Zurich Lake (n.s.i.): at surface: 6 ng/L; at 30-m depth: 42 ng/L
in tap water (Zurich): (n.s.i.) 4 ng/L (513)
In Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 9.6 mg/kg of organic carbon
suspended sediments: 0.49 mg/kg of organic carbon
water: 12 ng/L (2646)
In rivers in U.K. (1986): 139 samples from 70 river sites yielded 2 positive values (detection limit: 0.1 µg/L): median of positive values: 0.2 µg/L; maximum: 0.22 µg/L. (2711)

Soil sorption: log K_{oc}: 3.87. (2597)

D. BIOLOGICAL EFFECTS:

Residues: in fat phase of the following fish from the Frierfjord (Norway), April 1975–Sept. 1976: cod, whiting, plaice, eel, sprot:
average: 0.5 ppm (sum of all isomers)
range: 0.1–1.5 ppm (sum of all isomers) (1065)

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*

Bacteria: *Siderocapsa treubii*	200		(1833)
Insects: *Chironomus riparius,* 3rd instar larvae	9.6	wet wt	
	1,800	lipid wt	(2713)
Algae: *Myriophyllum spicatum* 0.35	33	total plant	
	16,000	lipid basis	(2560)
Crabs: blue crab	58.900	lipid	
Fishes: Atlantic croakers	34,700	lipid	
spotted sea trout	1,350	Lipid	
blue catfish	30,900	Lipid	
rainbow trout	14,000-29,500	lipid	
guppy	645		(2646)

INSECTS:

Chironomus riparius, 3rd instar larvae	48h LC_{50}	1.7 mg/L	
	48h LC_0	1.4 mg/L	
	48h LC_{100}	2.1 mg/L	
	48h NOLC	1.1 mg/L	
	48h NOEC	0.34 mg/L	(2713)

WORMS:
Biouptake by Oligochaete worms Tubifex tubifex *and* Limnodrilus hoffmeisteri: worm/sediment cumulation factor after 79 d at 8°C and 0.23 mg/kg sediment: 0.4; $t_{1/2}$ in worm: <5 d. (2618)

EARTHWORMS: LBB: 2.1 µmol/g wet wt (2715)

FISHES:
In catfish:

Bayou d'Inde industrial outfall:	0.77 mg/kg of lipid
junction of Bayou d'Inde and Calcasieu River:	0.37 mg/kg of lipid
Lake Charles:	not detect. mg/kg of lipid

Toxicity:

EARTHWORMS:
Eisenia andrei: 14d LC_{50}: 12–17 µg/L (estd. conc. in the soil pore water phase) (2789)
Lumbricus rubellus: 14d LC_{50}: 14–17 µg/L (estd. conc. in the soil pore water phase) (2789)

FISHES:

guppy *(Poecilia reticulata)*	14d LC_{50}	2.4 mg/L	(1833)
	4d LC_{50}	0.35 mg/L	(2625)

1,2,4-trichlorobenzene

$C_6H_3Cl_3$

CAS 120-82-1

USES: solvent in chemical manufacturing; dyes and intermediates; dielectric fluid; synthetic transformer oils; lubricants; insecticides.

A. PROPERTIES: colorless crystals or clear liquid with aromatic odor; molecular weight 181.46; melting point 17°C; boiling point 213°C; density 1.57 at 10/4°C; vapor pressure: 0.00045 atm at 20°C, 0.22-0.36 hPa at 20 °C; 0.8 hPa at 30 °C; 2.7 hPa at 50 °C; vapor density 6.25; solubility 19 mg/L at 22°C, 36 mg/L at 20 °C; log O_{oct}: 3.97; 4.0; 4.23; 4.52; H 108 Pa m^3/mol.

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.13 ppm, 1 ppm = 7.54 mg/m^3. (65)

Air quality: indoor/outdoor glc's winter 1981/1982 and 1982/1983, the Netherlands:

	µg/m³ median	µg/m³ maximum	
pre-war homes	<0.8	5	
post-war homes	<0.8	15	
homes <6 years old	<0.8	33	
outdoors	<0.8	<0.8	(2668)

Incinerability:
Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 955°C.
Thermal stability ranking of hazardous organic compounds: rank 26 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

Manmade sources: in municipal landfill gases in S. Finland (1989–1990): avg <0.05–0.07, max 0.13 mg/m³. (2605)

C. WATER POLLUTION FACTORS:

Manmade sources:
Göteborg (Sweden) sew. works 1989–1991: infl.: 0–1.0 µg/L; effl.: n.d. (2787)
Occurrence in sewage sludges, NW England 1989:

urban	mean	111 µg/kg dry wt	
	SD	200 µg/kg dry wt	
urban/industrial	mean	476 µg/kg dry wt	
	SD	453 µg/kg dry wt	(2953)

Water and sediment quality:
In Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 306 mg/kg of organic carbon
suspended sediments: 4.9 mg/kg of organic carbon
water: 40 ng/L (2646)
In rivers in U.K. (1986): 139 samples from 70 river sites yielded 4 positive values (detection limit: 0.1 µg/L): median of positive values: 0.16 µg/L; maximum: 0.3 µg/L. (2711)

Biodegradability: degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.07 mg/L: 50% removal in less than 4 d; 62% removal in 32 d. Biodegradation may have been the mechanism of removal for part or all of the reductions observed. (2653)
anaerob. digest. sew. sludge from municipal area U.K. 1989: mean: 40 µg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area U.K. 1990: mean: 351 µg/kg (2688)

Disappearance in a BOD test (BOD Die-AwayTest):

	at 1.7 mg/L TCB		at 2.6 mg/L TCB	
		% by GC-EC		% by GC-EC
days	*% ThOD*	*analysis*	*% ThOD*	*analysis*
1	14		0	
3	36		0	
5	37	0	23	
7	43		28	
10	55	99	19	100
20	55		55	(2692)

Activated sludge: after 120 h, 1,2,4-TCB was distributed as follows:
56% was converted to CO_2
7% had volatilized as TCB
23% was converted to polar metabolites
13% remained as 1,2,4-TCB, of which 80% was adsorbed on solids and 20% remained in the water (2692)

Biodegradation at 0.1 mg/L:

	normal sewage	adapted sewage	
after 24 h	0%	22%	
after 135 h	0%	56%	(997)

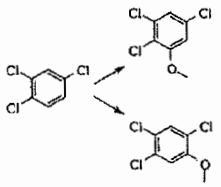
Biodegradation: degradation by *Pseudomonas:* 200 mg/L at 30°C
parent: 92% ring disruption in 120 h
mutant: 100% ring disruption in 46 h (152)

Fate of ^{14}C-labeled compound in a laboratory soil-plant system (7 d):

volatilization	23%
mineralization	0.46%
soluble metabolites in soil	0.28%
bound residues	3.5%
uptake by barley	0.54%
uptake by cress	0.47%

(2616)

Conversion products isolated from soil:

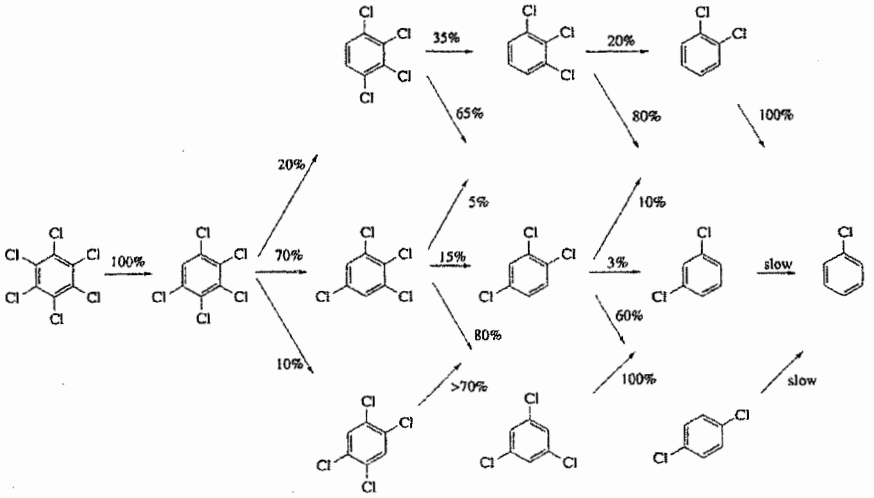


(2616)

Biodegradation

Inoculum	*method*	*concentration*	*duration*	*elimination results*	
A.S.	Modified MITI Test	100 mg/L	14 d	0% ThOD	(8890)

Reductive dechlorination in sediment under sulfate reducing conditions at 25 °C: half life period assuming peudo first order kinetics: 41 d . (7041)



Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

Impact on biodegradation processes: BOD test is inhibited from 5 mg/L onward. (30)

Effect on respiration of glucose by mixed culture derived from activated sludge:

concentration, mg/L	*increase in lag period, h*	*respiration rate, %*	
1	10	94	
10	0	71	
100	0	47	
1,000	>200	0	(997)

Reduction of amenities: T.O.C. = 0.005 mg/L. (225)

Soil sorption:

log K_{oc}: 3.83 (2597)

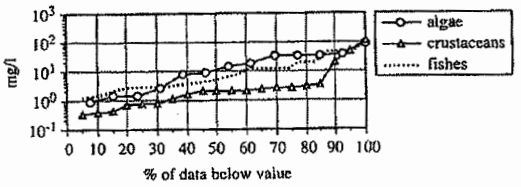
2050 1,2,4-trichlorobenzene

K_{oc}:	for Fullerton soil, 0.06% OC	1,300	
	for Apison soil, 0.11% OC	2,100	
	for Dormont soil, 1.2% OC	885	(2599)

D. BIOLOGICAL EFFECTS:

Bioaccumulation	*Concentration µg/L*	*exposure period*	*BCF*	*organ/tissue*	
Algae: *Chlorella fusca*			250	wet wt	(2659)
Crab: blue crab			79,000	lipid	
Fishes: Atlantic croaker			58,000	lipid	
spotted sea trout			3500	lipid	
blue catfish			48,000	lipid	
rainbow trout:			15,000-36,000		(2646)
fathead minnow			400-2,000		
rainbow trout	0.006		2,300-3,700		(2399, 2400)
	0.0005		1200		(2400)
Cyprinus carpio	5	42 d	120-1320	total body	
	50	42 d	1,140-4,420	total body	(8890)

PLANTS:			
Lactuca sativa R2	7d EC_{50}	56 mg/kg soil	
	14d EC_{50}	48 mg/kg soil	(8897)
BACTERIA:			
Activated sludge respiration inhibition	EC_{50}	500 mg/L	(2624)
A.S. oxygen consumption inhibition	15h EC_{50}	7,700 mg/L	(8896)
methanogens	48h IC_{50}	120 mg/L	(8896)
Nitrosomonas	24h IC_{50}	210 mg/L	(8896)
Pseudomonas putida	30min EC_{10}	>30 mg/L	(8892)
Photobacterium phosphoreum	5min IC_{50}	2.3 mg/L	(8896)
ALGAE:			
Tetrahymena pyriformis growth inhibition	24h EC_{50}	0.91 mg/L	
Chlorella vulgaris	7d EC_{50}	5.6 mg/L	(8893)
Selenastrum capricornutum	96h EC_{50}	37 mg/L	(8892)
DIATOMS:			
Cyclotella meneghiniana (DNA reduction)	48h EC_{50}	2.8 mg/L	(8898)
WORMS:			
Tubifex	48h LC_{50}	24 mg/L	(2624)
CRUSTACEANS:			
Daphnia magna	EC_{50} reproduction	0.33 mg/L	
	NOEC reproduction	0.18 mg/L	
	NOEC growth	0.061 mg/L	
	LC_{50}	0.76 mg/L	(2706)



FISHES:			
killifish *(Oryzias latipes)*	48h LC_{50}	12 mg/L	(2624)
Cyprinodon variegatus	96h LC_{50}	21 mg/L	

1,300		early life stage	MATC	0.22 mg/L (2643)
2,100		guppy *(Poecilia reticulata)*	14d LC_{50}	2.4 mg/L (1833)
885	(2599)	*Cyprinodon variegatus*	96h LC_0	15 mg/L
			96h LC_{100}	2.2 mg/L (6100)
		Jordanella floridae	96h LC_{50}	1.2; 4.0 mg/L (8891)
		Lepomis macrochirus	24h LC_{50}	109 mg/L (8892)
		Leuciscus idus	48h LC_{50}	0.7 mg/L (8892)
	(2659)	*Oryzias latipes*	48h LC_{50}	4.9; 12 mg/L (8893, 8890)
			96h LC_{50}	4.8 mg/L (8893)
		Pimephales promelas	96h LC_{50}	2.8 mg/L (8894)
	(2646)	bluegill *Lepomis macrochirus*	24h LC_{50},S	13 mg/L
			96h LC_{50},S	3.4 mg/L (2697)
	(2399, 2400)			
	(2400)	MAMMALS:		
		rat	oral LD_{50}	1107; 1019; 930; 756; 855; 600; 550 mg/kg bw
	(8890)			

mg/kg soil			µg/L	*Lowest NOEC per species,*
mg/kg soil	(8897)	Bacteriophyta	4,500	47,000
		Chlorophyta	190	
		Mycophyta	59,000	
		Protozoa	5,800	
500 mg/L	(2624)	Branchiopoda	190	
		Malacostraca	960	
,700 mg/L	(8896)	Pisces	500	(2906)
120 mg/L	(8896)			
210 mg/L	(8896)			
>30 mg/L	(8892)			
2.3 mg/L	(8896)			

1,3,5-trichlorobenzene

0.91 mg/L

5.6 mg/L (8893)
37 mg/L (8892)

$C_6H_3Cl_3$

2.8 mg/L (8898)

CAS 108-70-3

A. PROPERTIES: long needles; molecular weight 181.46; melting point 64°C; boiling point 208.5°C; solubility 5.8 mg/L at 20°C; log P_{oct} 4.20.

24 mg/L (2624)

B. AIR POLLUTION FACTORS:

0.33 mg/L
0.18 mg/L
0.061 mg/L
0.76 mg/L (2706)

Air quality: indoor/outdoor glc's winter 1981/1982 and 1982/1983, the Netherlands:

	µg/m³ median	µg/m³ maximum	
pre-war homes	<0.8	<0.8	
post-war homes	<0.8	8	
homes <6 years old	<0.8	5	
outdoors	<0.8	<0.8	(2668)

Incinerability:
Temperature for 99% destruction at 2.0-sec residence time under oxygen-starved reaction conditions: 955°C.
Thermal stability ranking of hazardous organic compounds: rank 26 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

12 mg/L (2624)
21 mg/L

C. WATER POLLUTION FACTORS:

2052 1,3,5-trichlorobenzene

Manmade sources:
Occurrence in sewage sludges, NW England 1989:

urban	mean	4.5 µg/kg dry wt	
	SD	3 µg/kg dry wt	
urban/industrial	mean	18 µg/kg dry wt	
	SD	12 µg/kg dry wt	(2953)

anaerob. digest. sew. sludge from municipal area, U.K. 1989: mean: 2.4 µg/kg
anaerob. digest. sew. sludge from 60% municipal and 40% indust. area, U.K. 1990: mean: 41 µg/kg (2688)

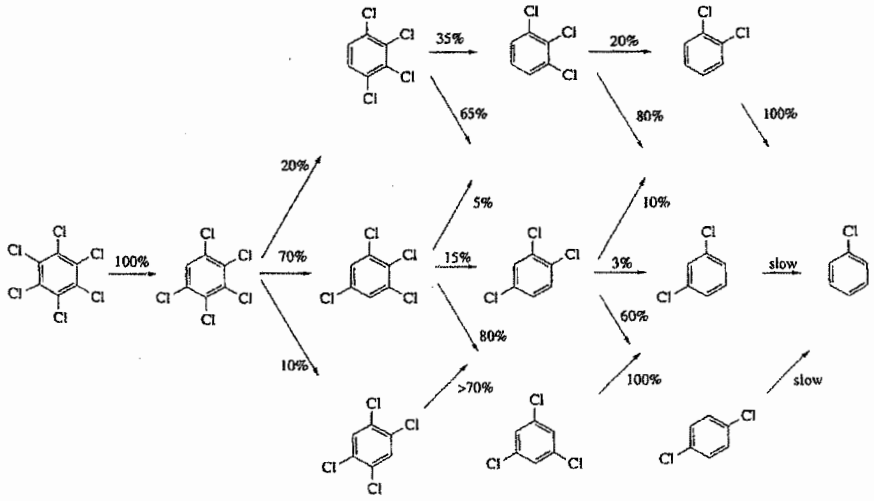
Water and sediment quality:
In Bayou d'Inde (Louisiana, U.S.A.) near industrial outfall:
bottom sediments: 83 mg/kg of organic carbon
suspended sediments: 0.96 mg/kg of organic carbon
water: n.d. (2646)
In rivers in U.K. (1986): 139 samples from 70 river sites yielded 5 positive values (detection limit: 0.1 µg/L): median of positive values: 0.18 µg/L; maximum: 0.3 µg/L. (2711)

Reduction of amenities: T.O.C. = 0.05 mg/L. (225)

Biodegradation:
degradation by *Pseudomonas:* 200 mg/L at 30°C
parent: 78% ring disruption in 120 h
mutant: 100% ring disruption in 50 h (152)
biodegradation at 1.0 mg/L:

	normal sewage	*adapted sewage*	
after 24 h	0%	20%	
after 135 h	0%	47%	(997)

Degradation during anaerobic sludge digestion at 37°C in a batch digester at initial conc. of 0.07 mg/L: 25% removal in 32 d. The removal must be attributed to a chemical conversion or physical removal process other than sorption. (2653)
Reductive dechlorination in sediment under sulfate reducing conditions at 25°C: half life period assuming peudo first order kinetics: 35 d. (7041)



Estimated dechlorination pathway of chlorobenzenes in a sulfate reducing anaerobic sediment (7041)

Soil sorption: K_{oc}: 700 at 0.5 mg/L. (2588)

D. BIOLOGICAL EFFECTS:

2142 2,4,6-trimethyl-1,3,5-trioxane

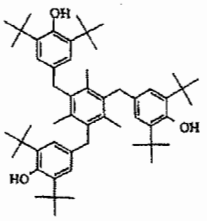
Manmade sources:
in effluents of 5 municipal sewage treatment plants: 0.5–5 ng Sn/L
in effluent of organotin production plant: 770 ng Sn/L
in the sediment of the Schwarzbach, a tributary of the Rhine near Mainz (Germany): 27,000 ng/kg dry wt (2419)

D. BIOLOGICAL EFFECTS:

Toxicity to microorganisms: growth inhib.	EC_{50}	3.7 mg/L	
Thymine incorporation inhib.	EC_{50}	17; 43 mg/L	(2624)
FISHES:			
Skeletonoma costatum	EC_{50}	0.21 mg/L	
Theulassiosira pseudonana	EC_{50}	0.35 mg/L (calculated)	(6153)
MAMMALS:			
rat	oral LD_{50}	12.6 mg/kg bw	(6164)

2,4,6-trimethyl-1,3,5-trioxane *see* paraldehyde

1,3,5-trimethyl-2,4,6-*tris*(3,5-di-*t*-butyl-4-hydroxybenzyl)benzene (ionox 330)



CAS 1709-70-2

USES: antioxidant in polyethylene, polypropylene, polystyrene, natural and synthetic rubber, lubricants, grease, etc.

A. PROPERTIES: molecular weight 775.22; melting point 244°C; solubility 1.2 mg/L.

C. WATER POLLUTION FACTORS:

BOD_5:	0.92 = 31% ThOD	
COD:	0.82 = 27% ThOD	(277)

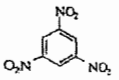
D. BIOLOGICAL EFFECTS:

FISHES: goldfish: LC_0 = 96h 1.2 mg/L (277)

1,3,7-trimethylxanthine *see* caffeine

trinitrin *see* nitroglycerine

1,3,5-trinitrobenzene (1,3,5-TNB)



$C_6H_3(NO_2)_3$

t (2419)

.7 mg/L

43 mg/L (2624)

21 mg/L
lculated) (6153)

ıg/kg bw (6164)

s, grease, etc.

(277)

(277)

$C_6H_3N_3O_6$

CAS 99-35-4

A. PROPERTIES: molecular weight 213.12; melting point 122°C; vapor pressure 3.03×10^{-6} torr at 25°C; solub 385 mg/L at 25°C; log P_{oct} 1.18.

B. AIR POLLUTION FACTORS:

Incinerability: thermal stability ranking of hazardous organic compounds: rank 183 on a scale of 1 (highest stability) to 320 (lowest stability). (2390)

C. WATER AND SOIL POLLUTION FACTORS:

Manmade sources: constituent of condensate water of TNT manufacturing process.
Soil sorption: log K_{oc}: 1.30.

D. BIOLOGICAL EFFECTS:

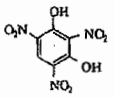
CRUSTACEANS: water flea	48h LC_{50}	2.7 mg/L	(2627)
FISHES: fathead minnow	96h LC_{50}	1.1 mg/L	(2627)

trinitroglycerine *see* nitroglycerine

2,4,6-trinitrophenol *see* picric acid

2,4,6-trinitrophenylmethylnitramine *see* tetryl

2,4,6-trinitroresorcinol (styphnic acid; 2,4-dihydroxy-1,3,5-trinitrobenzene)



$(HO)_2C_6H(NO_2)_3$

$C_6H_3N_3O_8$

CAS 82-73-5

A. PROPERTIES: yellow crystals; molecular weight 245.12; melting point 179–180°C.

C. WATER POLLUTION FACTORS:

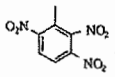
Waste water treatment: adapted culture: 7% removal after 48 h incubation, feed = 199 mg/L. (292)

D. BIOLOGICAL EFFECTS:

BACTERIA: *Pseudomonas putida*	16h EC_0	>100 mg/L	(329)
ALGAE:			
Microcystis aeruginosa	8d EC_0	0.32 mg/L	(329)
Microcystis aeruginosa	8d EC_0, growth	15 mg/L	(318)
Selenastrum capricornutum	8d EC_0	5 mg/L	
FISHES:	96h LC_{50}	2.6 mg/L	
	96h EC_{50}	0.46 mg/L, behavioral response	(318)

2144 2,3,6-trinitrotoluene

2,3,6-trinitrotoluene (2,3,6-TNT)



$CH_3C_6H_2(NO_2)_3$

$C_7H_5N_3O_6$

A. PROPERTIES: molecular weight 227.13.

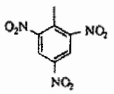
C. WATER AND SOIL POLLUTION FACTORS:

Manmade sources: constituent of condensate water of TNT manufacturing process.

D. BIOLOGICAL EFFECTS:

CRUSTACEANS: water flea	48h LC_{50}	0.8 mg/L	(2627)
FISHES: fathead minnow	96h LC_{50}	0.1 mg/L	(2627)

2,4,6-trinitrotoluene (TNT)



$CH_3C_6H_2(NO_2)_3$

$C_7H_5N_3O_6$

CAS 118-96-7

USES: explosive; intermediate in dyestuffs and photographic chemicals.

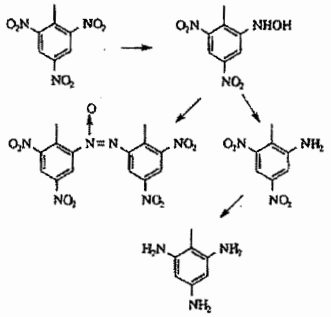
A. PROPERTIES: colorless to yellowish odorless crystals; molecular weight 227.13; melting point 80.7 °C; bp 240 °C explodes; vapor pressure 0,74 10^{-5} hPa at 20 °C, 5,7 100^{-2} hPa at 81 °C; vapor density 7.85; density 1.65; saturation concentration 0.038-0.089 mg/m^3 at 25 °C; solubility 200 mg/L at 15 °C, 140 mg/L at 25 °C; log P_{oct} 1.84, 1.86, 2.00; log *H* -5.96 at 25 °C (measured)

B. AIR POLLUTION FACTORS: 1 mg/m^3 = 0.11 ppm, 1 ppm = 9.44 mg/m^3.

Upon explosion the following gases are produced: carbondioxide, carbonmonoxide, water, nitrogen, methane, hydrogen, hydrogen cyanide and nitrogen oxides.

C. WATER POLLUTION FACTORS:

Biodegradation: self-purification of surface water is affected from 0.5 mg/L. (181)
Impact on treatment processes: biochemical oxidation is decreased from 0.5–1.0 mg/L onwards.
Microbial transformations:



During biological reduction nitroso-derivatives are formed as intermediate compounds Aerobic and anaerobic degradation by cultures of *E.Coli, Veillonella alkalescens* and *Pseudomonas.* (3999)
After composting, the majority of TNT and its metabolites was removed with the percolation water, 14% was accounted as "bound-residue". (3999)
After an incubation period of 65 d at an initial concentration of 80 mg/kg in a loamy soil, the following products could be identified: 3% TNT, 6% 4-amino-2,6-dinitrotoluene and 4% 2-amino-4,6-dinitrotoluene. The remainder 87% was further degraded or bound to the organic soil fraction. (3999)
Adapted *Pseudomonas fluorescens* produced, under laboratory conditions, the following metabolites: pyrogallol, phloroglycin and ammonia. (2627)
The fungus *Phanerochaete chrysosporium* mineralized 35% of the initial concentration in 18 d. (2627)

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-5.96 at 25

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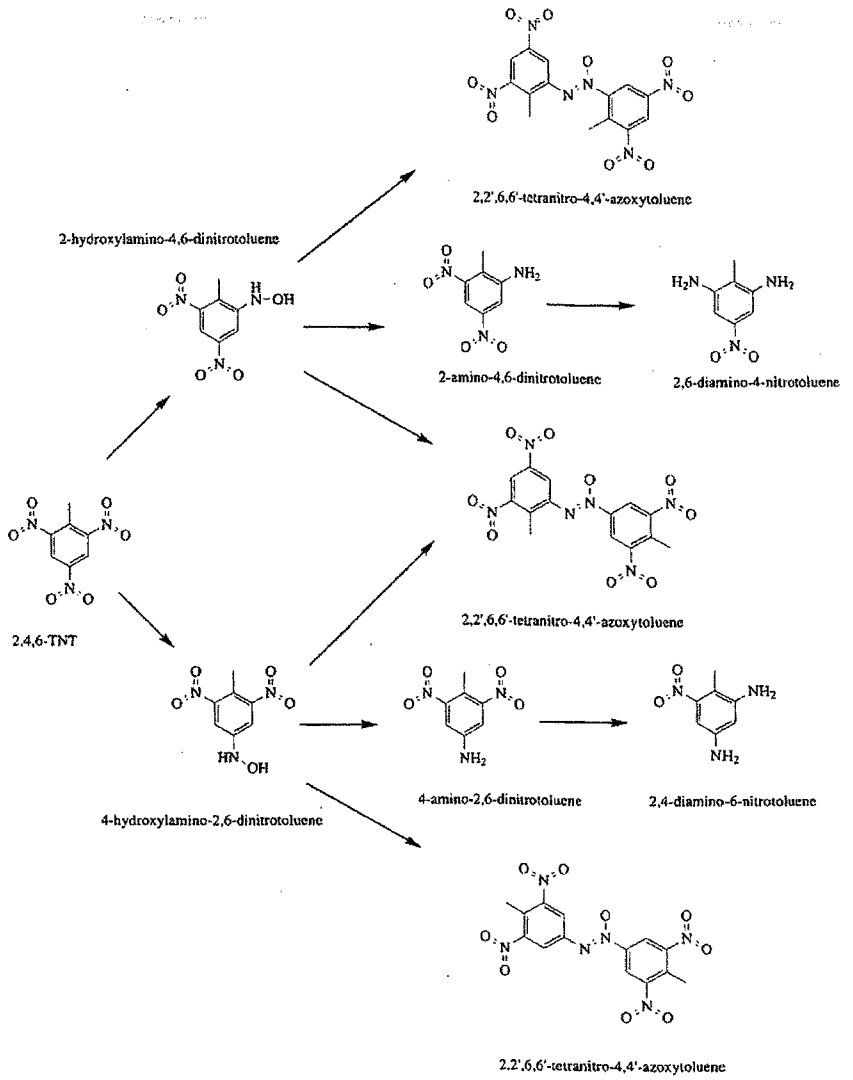
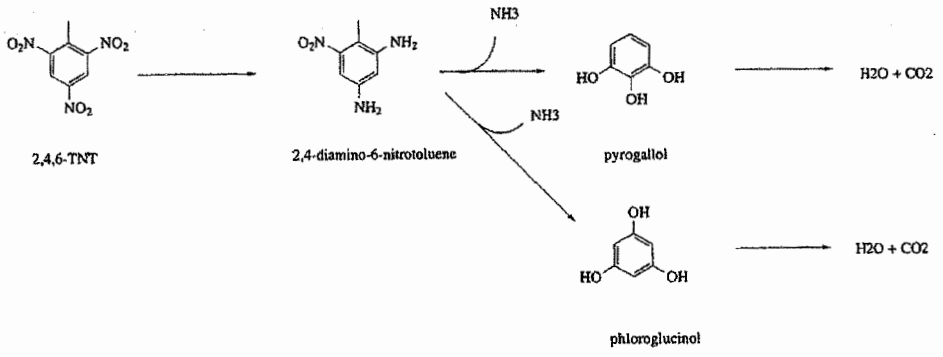
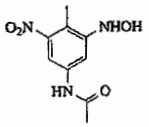


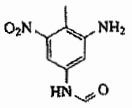
PATHWAYS OF TNT BIOTRANSFORMATION IN COMPOSTING



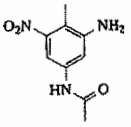
Biodegradation of 2,4,6-TNT in a laboratory experiment



4-N-acetylamino-2-hydroxylamino-6-nitrotoluene

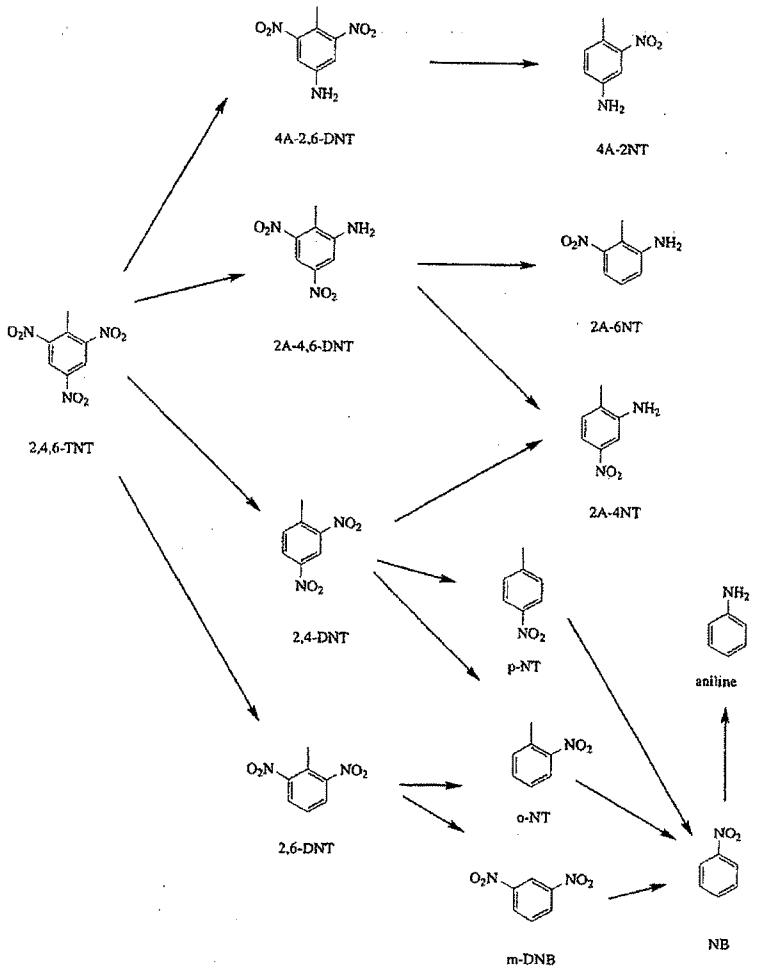


4-N-formylamino-2-amino-6-nitrotoluene



4-N-acetylamino-2-amino-6-nitrotoluene

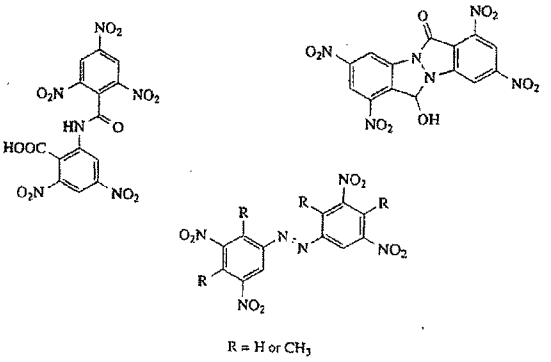
Identified acetylated and formylated TNT metabolites in anaerobic/aerobic compost (7079)



Metabolites of 2,4,6-TNT observed in polluted soil and groundwater of a former TNT production site.

TNT reacts with humic acids to form complexes. Half life time of TNT in the environment is 69 d. (3999)

Photolysis:



Phototransformation products of 2,4,6-TNT

Photolysis is the main degradation mechanism in shallow surface waters and in the upper layers of the soil. The following photolytic transformation prtoducts have been identified: 2,4,6-trinitrobenzylalcohol 2,4,6-trinitrobenzaldehyde 2,4,6-trinitrobenzaldoxime 2,4,6-trinitrobenzoic acid 2,4,6-trinitrobenzonitrile 1,3,5-trinitrobenzene 2-amino-4,6-dinitrobenzoic acid 2,2'-6,6'-tetranitro-4,4'-azoxytoluene 4,4'-6,6'-tetranitro-2,2'-azoxytoluene 2',4-dimethyl-3,3'-5,5'-tetranitro-ONN-azoxybenzene 2,4'-dimethyl-3,3'-5,5'-tetranitro-ONN-azoxybenzene 2-carboxy-3,3'-5,5'-tetranitro-ONN-azoxybenzene 2,2'-dicarboxy-3,3'-5,5'-tetranitro-ONN-azoxybenzene N-(2-carboxy-3,5-dinitrophenyl)-2,4,6-trinitrobenzamide 4,6-dinitroanthranile 2,4-dinitroisoanthranile 4,6-dinitroisoanthranile 3,5-dinitrophenol 4,6-dinitro-1,2-benzisoxazole
The photolytic $t_{1/2}$ = < 0.5 hours. (3999)

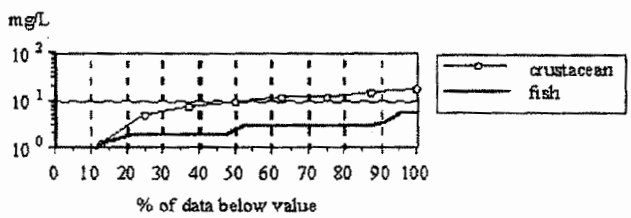
Soil sorption: log K_{oc}: 2.72; 3.2.

D. BIOLOGICAL EFFECTS:

Plants: the uptake capacity of plants is very large. Through the roots up to 75% of total TNT concentration can be absorbed. Very large differences have however been obeserved between plant species.

Toxicity threshold (cell multiplication inhibition test):

BACTERIA *(Pseudomonas putida):*	16h EC_0	>100 mg/L	(1900)
ALGAE *(Microcystis aeruginosa):*	8d EC_0	50 mg/L	(329)
GREEN ALGAE *(Scenedesmus quadricauda):*	7d EC_0	1.6 mg/L	(1900)
ALGAE *(Selenastrum capricornutum):*	7d EC_0	9 mg/L	(329)
PROTOZOA *(Entosiphon sulcatum):*	72h EC_0	1.6 mg/L	(1900)
PROTOZOA (*Uronema parduczi* Chatton-Lwoff):	EC_0	5.9 mg/L	(1901)



(3999)

FISHES:	96h LC_{50}	1.6 mg/L	
(behavioral response)	96h EC_{50}	0.64 mg/L	(318)
fathead minnow	96h LC_{50},F	2.6 mg/L (n.s.i.)	
(behavioral response)	96h EC_{50},F	0.46 mg/L (n.s.i.)	(473)

Acute toxicity under static conditions:

	exposure time, h	LC_{50} (mg/L) nonphotolyzed	photolyzed	
fathead minnow *(Pimephales promelas)*	96	2.9	13	
Channel catfish *(Ictalurus punctatus)*	96	2.4	5.5	
rainbow trout *(Salmo gairdneri)*	96	0.8	14	
bluegill *(Lepomis macrochirus)*	96	2.6	18	
water flea *(Daphnia magna)*	48	12	16	
scud *(Hyalella azteca)*	48	6.5	6.7	
midge *(Tanytarsus dissimilis)*	48	5.2	19	
earthworm *(Lumbricus variegatus)*	48	5.2	19	(2627)

Flow-through conditions: