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HANDBOOK OF TOXICOLOGY

VOLUME V
FUNGICIDES

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EDITOR

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PREPARED UNDER THE DIRECTION OF THE COMMITTEE
ON THE HANDBOOK OF BIOLOGICAL DATA

DIVISION OF BIOLOGY AND AGRICULTURE
THE NATIONAL ACADEMY OF SCIENCES
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FOREWORD

The Handbook of Toxicology, Volume V, Fungicides, is the ninth of a continuing series of publications*, each containing information, chiefly tabular, in one or more of the biological sciences. This book was prepared under Aero Medical Laboratory Contract No. AF 33(616)-2873 between the National Academy of Sciences-National Research Council and the Wright Air Development Center. The contract is administered under the direction of the Physiology Branch, Aero Medical Laboratory, Wright Air Development Center, with Dr. George Kitzes as project monitor. The work was performed under Project No. 7165, "Health Hazards of Air Force Materials and Radiation," Task No. 71836, "Evaluation and Control of Toxic Chemical Materials," under the direction of the Committee on the Handbook of Biological Data, operating under the Division of Biology and Agriculture of the National Academy of Sciences-National Research Council.

On behalf of the Committee, acknowledgement is made to the Wright Air Development Center, United States Air Force, to the National Institutes of Health of the Public Health Service, to the Division of Biology and Medicine of the Atomic Energy Commission, to the Office of Naval Research, to the Office of the Surgeon General of the Army, and to the Army Chemical Center, for generous support and cooperation which have made possible the production of this book. Special thanks go to Judith P. Bloomer and Nellie F. Brown for their untiring efforts in the drafting and typing of the manuscript.

*Handbooks published 1949-1959

Standard Values in Blood	1951
Standard Values in Nutrition and Metabolism	1953
Handbook of Toxicology, Vol. I, Acute Toxicities	1955
Handbook of Biological Data	1956
Handbook of Toxicology, Vol. II, Antibiotics	1957
Handbook of Respiration	1958
Handbook of Toxicology, Vol. III, Insecticides	1959
Handbook of Toxicology, Vol. IV, Tranquilizers	1959
Handbook of Toxicology, Vol. V, Fungicides	1959

ABSTRACT

This report summarizes data on 196 fungicides with regard to their physical, chemical, biological, and toxicological properties. An additional 500 compounds having fungicidal activity are listed in an appendix. These compounds have been compiled from an extensive review of 320 literature references. To enhance reliability and, consequently, usefulness, each page of data has been exhaustively reviewed and authenticated by the contributors.

The compilation is as complete as the rapid development of fungicides will permit. Wherever possible, data are presented on molecular formula and weight structure, physical and chemical properties, fungicidal tests, toxicity, and use. This report is offered not as a definitive work, but as the preliminary structure for a more exhaustive and better documented report. Corrections, suggestions, and additions would therefore be welcomed.

PUBLICATION REVIEW

This report has been reviewed and is approved.

FOR THE COMMANDER:

Andres I Karstens

ANDRES I. KARSTENS
Colonel, USAF (MC)
Ass't. Chief, Aero Medical Laboratory
Directorate of Laboratories

Contents

Volume V

Introduction

The term "fungicide," as herein used, includes any substance that destroys fungi, or inhibits their growth or reproduction. As befitting this series of Handbooks, selection of such substances for inclusion in Volume V was determined by the toxicological information available. A list of some 500 additional compounds with bibliographic references appears in Appendix II.

For the most part, compounds are presented according to the nomenclature of Chemical Abstracts. Deviation from this procedure occurs in the case of recent name changes, i.e., Fungicidin to Nystatin, with Fungicidin now the alternative name. For easy reference, the latter is included in the Index, as are all the more common alternative names for each compound.

Patent numbers, United States and foreign, are contained in Appendix I. Of the 196 compounds comprising this book, 112 are represented there.

With the exception of the structural formulas which were calculated from the Periodic Chart of the Elements, THE MERCK INDEX, Ed. 6, 1952 (Merck & Co., Inc., Rahway, N. J.), information for this volume has been gathered from the records of the Committee on Control of Deterioration and the Chemical-Biological Coordination Center of the National Academy of Sciences-National Research Council, as well as from the literature and from unpublished reports of experimental work on fungicides. A simple code (bracketed numbers) has been employed to indicate data source, with the full reference given in the Bibliography. So far as possible, literature citations conform to the LIST OF ABBREVIATIONS FOR SERIAL PUBLICATIONS, Fourth Series, 1948, Army Medical Library, Washington, D. C. (U. S. Government Printing Office), and the 1955 SUPPLEMENT thereto.

The material contained in this handbook has been examined for accuracy by the analysts and has also been reviewed by authorities in the field of pathology. It must be emphasized, however, that the data, particularly those concerned with toxicity, are not precise and should be interpreted only as indications of activity. This book is offered not as a definitive work, but as the preliminary structure for a more exhaustive and better-documented report. Corrections, suggestions, and additions would therefore be welcomed.

Abbreviations

Bibliographic

CBCC = Chemical-Biological Coordination Center
NAS = National Academy of Sciences
NIH = National Institutes of Health
NRC = National Research Council
PDC = Prevention of Deterioration Center

Dose

ED = effective dose
LC = lethal concentration
LD = lethal dose
ED_{50} = dose effective in 50% of an experimental group of organisms
LC_{50}, LD_{50} = concentration or dose lethal for 50% of a group of organisms
MED = minimum effective dose
MLD = minimum lethal dose
MTD = maximum tolerated dose

Route of Administration

c.t. = cutaneous
i.m. = intramuscular
i.p. = intraperitoneal
i.v. = intravenous
p.o. = oral
r.t. = rectal
s.c. = subcutaneous
s.t. = stomach tube

Measurement

da = day
hr = hour
min = minute

cc = cubic centimeter
L = liter
ml = milliliter

g = gram
kg = kilogram
mg = milligram
µg = microgram
M = mole

ppm = parts per million

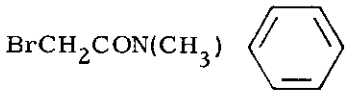
Fungicides

1. ACETANILIDE, 2-BROMO-N-METHYL-

ALTERNATIVE NAME (Bromoacetyl)methylaminobenzene.

MOLECULAR FORMULA $C_9H_{10}BrNO$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless prisms. Molecular weight, 227.984. Melting point, 48°C. Soluble, approximately 1:2, in acetone, benzene; "Cellosolve," approximately 1:4. Stable at room temperature. [48]

TESTS In vitro. Growth of inoculum (approximately 7.5×10^3 spores placed on treated slide for germination test) inhibited: Botrytis cinerea Fr., (0.65 µg/sq cm) 98-100%; Sclerotinia fructigena Aderh. and Ruhl., (0.65 µg/sq cm) 93-97%; Alternaria brassicae (Berk.) Sacc., (0.2-0.65 µg/sq cm) 0-50%. [49]

Growth of inoculum (1/8-inch, mycelial-covered cotton thread, rolled in 10% test compound in inert base of waterproof limestone powder) inhibited: Corticium solani (Prill. and Delacr.) Bourd. and Galz., Botrytis cinerea Fr., Fusarium nivale Auct., F. caeruleum (Lib.) Sacc., 98-100%; Helminthosporium avenae Eidam., 0-50%. [49]

TOXICITY LD_{50} in mice, approximately 60 mg/kg, p.o., in acacia. Skin irritation. [48]

USE Protectant of materiel.

2. ACETIC ACID, DICHLORO-

ALTERNATIVE NAMES Dichloroethanoic acid; 2,2-Dichloroacetic acid; Dichloroacetic acid; Urner's liquid.

MOLECULAR FORMULA $C_2H_2Cl_2O_2$

STRUCTURAL FORMULA $Cl_2CHCOOH$

2. ACETIC ACID, DICHLORO- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid. Pungent odor. [192] Molecular weight, 128.950. Melting point, -4°C. Boiling point, 193-194°C. Specific gravity, 1.5724 (13°C). [53] Soluble at 25°C in acetone, benzene, carbon tetrachloride, ether. Also soluble in water, alcohol, n-heptane, methanol. [118]

TESTS In vitro.

	µg/sq cm	% Inhibited
Stemphylium sarcinaeforme Cav.	1000	100
	100	41
	10	6
	1	0
Sclerotinia fructicola (Wint.) Rehm.	1000	93
	100	11
	10	0

[8]

Chaetomium globosum, and Aspergillus niger (Van Tiegham): 1% of test compound prevented infestation [64].

TOXICITY

Animal	LD_{50}, mg/kg	Route	Time of Death
Mouse	5520(3810-8000)	p.o.	36 hr
Rabbit	510(390-670)	c.t.	
Rat	4480(4290-4690)	p.o.	36 hr

[120]

COMPARATIVE TOXICOLOGY LD_{50} for dosage by mouth is of the same order of magnitude as the LD_{50} for acetic acid [250].

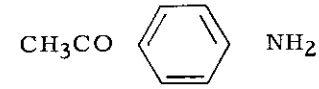
USE Medicinal.

3. ACETOPHENONE, p-AMINO-

ALTERNATIVE NAME p-Aminophenyl methyl ketone.

MOLECULAR FORMULA C_8H_9NO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow needles. Molecular weight, 135.160. Melting point, 106°C [118], 110°C (corr.) [228]. Boiling point, 205°C [118], 293-295°C [228]. Soluble in aqueous alcohol, boiling ether, boiling water. Slightly soluble in benzene, petroleum, ether. [228]

3. ACETOPHENONE, p-AMINO- (Concluded)

TESTS In vitro. Aspergillus niger (Van Tiegham): 1 drop of spore suspension and 250 ppm of test compound in nutrient-toxic-agar, incubated 96 hours at 30°C. Growth inhibited 69%. [229]

TOXICITY LD_{50} in mice, 465 ± 19 mg/kg, i.p. [120]. In male mice given i.p. injection of test compound dissolved in water or propylene glycol, 10 out of 10 survived 200 mg/kg, 1 out of 8 died after 300 mg/kg, 8 out of 8 after 400 mg/kg; observation period, 10 days. [280]

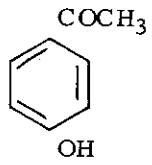
USE Protectant of materiel.

4. ACETOPHENONE, 4'-HYDROXY-

ALTERNATIVE NAME p-Hydroxyacetophenone.

MOLECULAR FORMULA $C_8H_8O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 136.144. Melting point, 103°C [69], 109°C [153]. Boiling point, 147-148°C (3 mm Hg). Specific gravity, 1.109 [153]. Soluble at 25°C in water, acetone, carbon tetrachloride, methanol, benzene, ether, VMP naphtha [69]. Very soluble in alcohol [153].

TESTS In vitro. Spores of Stemphylium sarcinaeforme Cav., and Monilinia fructicola: ED_{50}, 1000 µg/sq cm. [138]

In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 5% solution of test compound, dried, and stored at 70°F for 3 weeks. Decay prevented; no rind injury. [294]

TOXICITY Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight; exposure 24 hours. No injury. [291]

USE Protectant of materiel.

5. ACRYLONITRILE

ALTERNATIVE NAMES Vinyl cyanide; Propenenitrile; Cyanoethylene.

MOLECULAR FORMULA C_3H_3N

STRUCTURAL FORMULA $CH_2=CHCN$

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]. Mild odor [53]. Molecular weight, 53.062. Freezing point, -82°C [118], -83.71°C [70]. Boiling point, 73.97°C [70], 75-77°C [228], 78-79°C [118]. Vapor pressure, 114.3 mm Hg (25°C) [70]. Specific gravity, 0.80848 [70], 0.797 [118]. Refractive index, 1.39093 [70], 1.393 [118]. Soluble in water [228]. Miscible with acetone, carbon tetrachloride, benzene, ether, n-heptane, alcohol [70].

TOXICITY Man. Inhalation causes nausea, vomiting, diarrhea, weakness, headache, and jaundice. Skin contact causes blistering. [71] Erythema and painful blisters of skin [101]. Flushing of face, increased salivation irritation of eyes and nose; respiration at first rapid and deep, then shallow [250]. Weakness, light-headedness, headache, nausea, sneezing, abdominal pain, vomiting, loss of consciousness, asphyxia, death [192].

Animals. LD in rats, 635 ppm. LD in dogs, 110 ppm. [180]

Animal	Dose	mg/kg	Route	Reference
Guinea pig	LD_{50}	50	p.o.	120
Mouse	LD_{50}	15	i.p.	120
Mouse	LD	>20, <72	p.o.	47, 120
Rabbit	LD_{50}	250	c.t.	120
Rabbit	LD_{50}	25	Skin absorption	47
Rat	LD_{50}	93(81-106)	p.o.	120

Animal	Dose	mg/L	ppm	Exposure Time	Time of Death
Dog	MLC	0.24	110	Continuous	4 hr
Rat	LC_{50}	1.1	500	4 hr	
Rat	MLC_{100}	1.38	635	4 hr	8 hr

[120]

USE Protectant of materiel: textiles (mildew resistance).

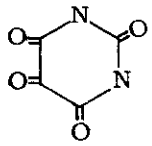
CAUTION Fumes are toxic; flammable. [53]

6. ALLOXAN

ALTERNATIVE NAMES Pyrimidinetetrone; Mesoxalylurea.

MOLECULAR FORMULA $C_4H_2N_2O_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Dark yellow (anhydrous), or colorless (hydrous), rhombic prisms. Molecular weight, 142.072. Decomposes, 170°C. Very soluble in water. Soluble in alcohol. [118]

TESTS In vitro. 10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours.

	µg/sq cm	% Inhibition
Stemphylium sarcinaeforme Cav.	1000	100
	100	100
	10	100
	1	64
Sclerotinia fructicola (Wint.) Rehm.	1000	100
	100	52

[55]

Aspergillus niger: 20 ppm inhibited growth 5%; 10 ppm, 5% [228].

TOXICITY

Animal	Dose	mg/kg	Route	Time of Death
Dog	MLD	100	i.v.	Few hr
Dog	LD	75-100	i.v.	1 wk
Mouse	LD_{50}	300-400	i.p.	48 hr
Mouse	LD_{50}	200	i.v.	48 hr
Rabbit	MLD	180-250[1]	r.t.[2]	
Rat	LD	300	i.v.	Rapid
Sheep	LD	200	i.v.	24 hr
Duck	MLD	250[3]	i.v.	36-48 hr
Pigeon	LD	150-200	i.v.	2-3 da

[120]

USE Protectant of materiel.

/1/ As alloxan monohydrate, 15% suspension in water. /2/ Or by injection into jejunum. /3/ 5% solution.

7. ALTERNARIC ACID

SOURCE Alternaria solani (Ell. and Mart.) J. and G.

MOLECULAR FORMULA $C_{21}H_{30}O_8$

PHYSICAL AND CHEMICAL PROPERTIES Thin, colorless, rectangular plates or elongated prisms. Molecular weight, 410.550. Melting point, 138°C. Soluble in ethanol, methanol, pyridine, chloroform, benzene, ether, carbon tetrachloride. Slightly soluble in cold water. Insoluble in petroleum ether. [121] Stable to boiling 5 minutes at pH 3-7.6; partial loss of activity observed after autoclaving at pH 3.0.

TESTS In vitro. Compound active in these tests only at pH 3.5. Minimum concentration required to inhibit spore germination:

	µg/ml
Myrothecium verrucaria (Alb. and Schw.) Ditmer ex Fries	0.1
Mucor mucedo Bref.	0.4
Absidia glauca Hagen	0.8
Thamnidium elegans Link	0.8

Minimum concentration required to cause stunting of length of germ tubes and hyphal extension after germination and formation of germ tubes:

	µg/ml
Mucor mucedo Bref.	0.001
Thamnidium elegans Link	0.005
Botrytis allii Munn	0.01
Myrothecium verrucaria (Alb. and Schw.) Ditmer ex Fries	0.01
Stemphylium sp	0.04
Absidia glauca Hagen	0.1
Aspergillus tomarii Kita	3.1

[48]

Tests at pH 6.5 proved inactive at comparable concentration levels with the following organisms: Botrytis allii Munn, Fusarium graminearum Schwabe, F. caeruleum (Lib.) Sacc., Penicillium brevicompactum Dierckx, P. digitatum Sacc., Myrothecium verrucaria (Alb. and Schw.) Ditmer ex Fries.

Spore germination of Absidia glauca and Myrothecium verrucaria inhibited at concentrations of 0.1-1.0 µg/ml; Botrytis allii at 10.0 µg/ml [121].

PHYTOTOXICITY Toxic to radish, cabbage, carrot and tomato seedlings in concentrations of 1-10 µg/ml. May be the chemical agent directly responsible for the disease effects of early blight of potatoes. A crystalline toxin isolated from Alternaria solani filtrates, apparently identical with alternaric acid, produced wilting, epinasty and necrosis in tomato cuttings within a few hours, in dilutions as high as 1:50,000,000. [121]

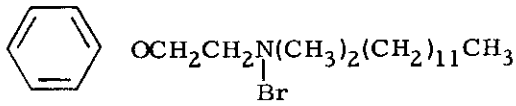
USE Medicinal.

8. AMMONIUM BROMIDE, DODECYLDIMETHYL(2-PHENOXYETHYL)-

ALTERNATIVE NAMES PDDB; Phenoxy-ethyl-dimethyl-dodecyl-ammonium bromide.

MOLECULAR FORMULA $C_{22}H_{40}NO^{+}\cdot Br^{-}$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 414.464.

TESTS In vitro. Culture media containing solutions of various concentrations of test compound, incubated 24 hours at 37°C. Maximum dilution capable of completely inhibiting growth:

	Dilution
Candida albicans	1:96,000
Torula lactosa	1:96,000
Trichophyton interdigitale	1:192,000
T. gypseum	1:96,000
Microsporum audouini Gruby	1:96,000
Aspergillus niger (Van Tiegham)	1:48,000
Penicillium notatum	1:96,000

[162]

TOXICITY

Animal	LD_{50}, mg/kg	Route
Guinea pig	10-20	i.p.
Mouse	31	i.v.
Rabbit	11-15	i.v.
Rat	40-45	i.p.
Rat	18	i.v.

[120]

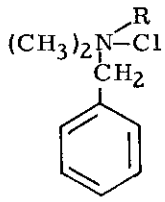
USE Medicinal.

9. AMMONIUM CHLORIDE, ALKYLBENZYLDIMETHYL-

ALTERNATIVE NAMES Roccal; Germ-I-tol [125]; Zephiran [302]; Zephirol; Benzalkonium chloride.

9. AMMONIUM CHLORIDE, ALKYLBENZYLDIMETHYL- (Concluded)

STRUCTURAL FORMULA



R = alkyls from C_8H_{17} to $C_{18}H_{37}$

PHYSICAL AND CHEMICAL PROPERTIES White, or yellow-white, amorphous powder or gelatinous pieces. Almost odorless. Bitter taste. Soluble in water, alcohol, acetone. Slightly soluble in benzene. Insoluble in ether. Alkaline to litmus. [302]

TESTS In vitro. Aspergillus niger (Van Tiegham): 0.0038% of test compound in medium (yeast extract, peptone, glucose, or potassium phosphate, at pH 6-7). Growth inhibited. [181]

TOXICITY Man. Dilutions below 1:1000 may cause skin irritation [250]. Probable LD, 50-500 mg/kg [101]. Principal manifestations are vomiting, collapse, coma [69].

Animals. LD_{50} in rats, 234.3 ± 26.5 mg/kg, s.t. [3]. Rabbits tolerated 0.12 cc/kg of a 10% solution [250].

Animal	Per cent in Diet	Mortality	Time of Death
Dog	1	2/2	7-12 wk
Dog	0.5	1/1	15 wk
Rat	0.5	50%	50 da
Rat	0.25	0%	2 yr

[3]

USE Protectant of materiel: paper [227]. Medicinal [105, 192].

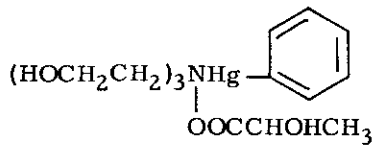
CAUTION Handlers should be equipped with rubber gloves, aprons, goggles [250].

10. AMMONIUM LACTATE, TRIS(2-HYDROXYETHYL)(PHENYLMERCURI)-

ALTERNATIVE NAME Phenylmercury triethanol ammonium lactate.

MOLECULAR FORMULA $C_{12}H_{20}HgNO_3^{+}\cdot C_3H_5O_3^{-}$

STRUCTURAL FORMULA



10. AMMONIUM LACTATE, TRIS(2-HYDROXYETHYL)(PHENYLMERCURI)- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White crystals. Molecular weight, 515.968. Melting point, 126°C. Soluble in water [92]. Unstable in reducing agents and sunlight [56]

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in saturated solution of test compound, dried, and stored 3 weeks at 70°F. Decay prevented; moderate rind injury. [291]

Sclerotinia laxa: Detached almond twigs at flowering stage and bearing sporodochia, sprayed with test compound and kept in moist chamber 3-8 days; conidia separated by crushing; plated, and incubated. 0.12% produced 56-75% mortality. Spraying trees in orchard did not control disease. [323]

TOXICITY Man. Highly toxic. Probable LD, 5-50 mg/kg [101]. Skin irritant and sensitizing agent [56].

Animals. LD_{50} in rats, 30 mg/kg, p.o. [56, 92, 120]. Seed treated with compound should not be fed to livestock [56].

COMPARATIVE TOXICOLOGY Systemic toxicity from test compound is almost as high as that caused by mercuric chloride, but corrosive effects are less [101].

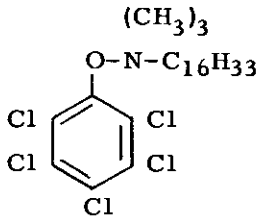
USE Protectant of materiel: textile preservative [227]. Agricultural: effective on apple leaves infected with Venturia inaequalis [126].

11. AMMONIUM PENTACHLOROPHENATE, HEXADECYLTRIMETHYL-

ALTERNATIVE NAMES Trimethylcetyl ammonium pentachlorophenate; Hexadecyl trimethyl ammonium pentachlorophenate.

MOLECULAR FORMULA $C_{25}H_{42}Cl_5NO$ or $C_{19}H_{42}N^+ \cdot C_6Cl_5O^-$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light brown paste. Molecular weight, 549.629. Melting point, approximately 68°C; fluid at 80°C. Not very stable in light.

11. AMMONIUM PENTACHLOROPHENATE, HEXADECYLTRIMETHYL- (Concluded)

TESTS In vitro. Spores of Stemphylium sarcinaeforme: LD_{50}, 3.75 µg/sq cm. Spores of Monilinia fructicola: LD_{50}, <1 µg/sq cm. [138]

Chaetomium globosum, Myrothecium verrucaria (Metarrhizium glutinosum), Aspergillus niger: Minimum inhibiting concentrations, 0.25% on yarn, 1% on duck cloth, 2% on sheeting. Bandolier cloth treated with 0.8% of compound was resistant to mold even with primary leaching, but was not resistant during soil burial. A solution of 0.25% on yarn was resistant to A. niger during soil burial for 21 days. [314]

TOXICITY Man. Skin irritation; 2.5% in sheeting in contact with skin approved by Surgeon General.[1] [300]

PHYTOTOXICITY Serious injury to tomato foliage in greenhouse [138].

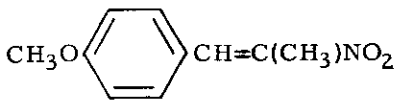
USE Protectant of materiel: mildew-proofing agent [125].

12. ANETHOLE, β-NITRO-

ALTERNATIVE NAME p-Methoxy-β-methyl-β-nitrostyrene.

MOLECULAR FORMULA $C_{10}H_{11}NO_3$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 193.196.

TESTS In vitro. Antifungal activity against Trichophyton (gypseum) mentagrophytes as determined by the agar diffusion plate method:

Concentration, M	Inhibition Zone, cm
1×10^{-2}	Complete
5×10^{-3}	Complete
1×10^{-3}	Complete
5×10^{-4}	8.0
1×10^{-4}	7.1
5×10^{-5}	5.7
1×10^{-5}	4.6
5×10^{-6}	4.5
1×10^{-6}	4.6

/1/ In another report, Surgeon General approved concentration of 2.5% for thread only.

12. ANETHOLE, β-NITRO- (Concluded)

Fungi	Time of Exposure	mg/ml[1]					
		10	1	0.1	0.01	0.001	0.0001
Candida albicans	Immediate	-	+	+	+	+	+
	15 min	-	-	+	+	+	+
	30 min	-	-	+	+	+	+
Cryptococcus neoformans	Immediate	-	-	+	+	+	+
	15 min	-	-	-	+	+	+
	30 min	-	-	+	+	+	+
Trichophyton mentagrophytes	Immediate	-	-	-	-	+	+
	15 min	-	-	-	-	+	+
	30 min	-	-	-	-	+	+
Blastomyces dermatitidis	Immediate	-	-	-	+	+	+
	15 min	-	-	-	-	+	+
	30 min	-	-	-	-	+	+

[26]

USE Medicinal.

13. ANTIMYCIN A

SOURCE Streptomyces spp [192].

MOLECULAR FORMULA $C_{28}H_{40}N_2O_9$

PHYSICAL AND CHEMICAL PROPERTIES Colorless crystals [53, 121]. Molecular weight, 548.616. Melting point, 139-140°C. Freely soluble in alcohol, ether, acetone, chloroform. Slightly soluble in benzene, carbon tetrachloride, petroleum ether. Insoluble in water. [53] Thermostable; stable at room temperature, less so at alkaline pH. [121]

TESTS In vitro. Inhibits Nigrospora sphaerica in a dilution of 1:8 x 10^8 [31].

	Inhibition, μg/ml
Colletotrichum spp	0.8-12.5
Nigrospora sphaerica	0.2
Phoma lingam	0.4
Chalara quercina	0.8
Sclerotinia fructicola	0.4-1.6
Venturia inaequalis	0.4-0.8
Stemphylium sarcinaeforme	1.6
Alternia kikuchiana	<1.0
Gloeosporium cingulata	<1.0
Gibberella saubinetti	<1.0

(continued)

/1/ (-) = no growth on subculture; (+) = growth on subculture.

	Inhibition, μg/ml
Ceratostomella fimbriata	<1.0
Sclerotinia arachidis	<1.0
Colletotrichum lindemuthianum	<1.0
Gloeosporium kaki	<1.0
Piricularia oryzae	<1.0-10
Cladosporium fulvum	10.0

Torula utilis sensitive to 0.1 μg/ml. Candida albicans, Aspergillus oryzae, A. niger, Trichophyton sp, not sensitive to 100 μg/ml [121].

TOXICITY

Animal	Dose	mg/kg	Route	Reference
Mouse	LD_{50}	21.2	s.c.	121
Mouse	LD_{50}	7.6	i.p.	121
Mouse	LD_{50}	0.9	i.v.	121
Rat		121,2	p.o.	121
Rat	LD	301	p.o.	121
Rat	LD_{50}	0.81	i.p.	47, 121

PHYTOTOXICITY Low toxicity in wide variety of plants [121].

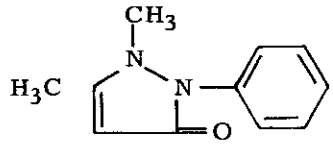
USE Medicinal. Agricultural [192]: effective in control of certain Helminthosporium diseases of oats and barley [121].

14. ANTIPYRINE

ALTERNATIVE NAMES Phenazone; Phenyldimethylpyrazolone.

MOLECULAR FORMULA $C_{11}H_{12}N_2O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals. Molecular weight, 188.222. Melting point, 112°C [69], 110-113°C [53]. Boiling point, 319°C (114 mm Hg). Specific gravity, 1.19. Soluble in water, alcohol, chloroform. Slightly soluble in ether. [53] Stable [69]. Neutral pH [154].

/1/ In methyl laurate. /2/ Tolerated.

14. ANTIPYRINE (Concluded)

TESTS In vitro. Aspergillus niger (Van Tiegham): Drop of spore suspension and 250 ppm of test compound in nutrient-toxic-agar; incubated 96 hours at 30°C. Growth inhibited 10%. [229]

Drop of test compound dried in depression slide cavity, spore suspension added; incubated 17 hours. Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm stopped germination. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm did not inhibit spore germination. [53]

TOXICITY Man. Probable LD, 50-500 mg/kg. Skin rashes common and persisting for several weeks. [101] Granulocytopenia, muscular twitching, skin eruptions, cyanosis, excitement, weakness, drowsiness, dyspnea, cold perspiration, pallor, anemia, rapid and feeble pulse, diminished urine volume, delirium, convulsions, respiratory failure, death [154]. Fatalities from acute poisoning are rare. Principal manifestations, mental disturbance and leukopenia [71].

Animals.

Animal	Dose	mg/kg	Route
Cat	LD	700	s.c.
Dog	LD	500-1000	p.o.
Guinea pig	LD	1400	p.o.
Guinea pig	LD	1000	s.c.
Mouse	LD	1000	s.c.
Rabbit	LD	1000-1500	s.c.
Rabbit	LD	600-800	i.v.
Rat	LD_{50}	1800	p.o.
Frog	LD	2000-4000	s.c.

[120]

COMPARATIVE TOXICOLOGY Less toxic than acetanilide [101].

USE Protectant of materiel.

15. ASCOSIN

SOURCE Streptomyces canescus.

PHYSICAL AND CHEMICAL PROPERTIES Not yet isolated in pure form. Crude preparations soluble in aqueous pyridine and other N-containing heterocyclic solvents. Slightly soluble in dry pyridine, most other organic solvents, water. Thermo-, acid, and alkali labile. [121]

TESTS In vitro. Inhibits the following yeasts and filamentous fungi:

	µg/ml
Candida albicans	0.2
C. krusei	0.4
Torula utilis	0.4
Willia sp	0.8
Aspergillus niger	1.6
Saccharomyces cerevisiae	1.6
Absidia orchidis	6.2
Botrytis sp	6.2
Trichophyton interdigitale	25
Mucor pusilis	50

Also inhibits Mycoderma, Cryptococcus, Histoplasma capsulatum, Penicillium spinulosum, Rhizopus nigricans [121].

Test organisms, cultured in presence of compound dissolved in aqueous pyridine, buffer, or saline on Difco phenol red broth, and incubated for 24 hours at 28°C, are listed according to the minimal concentration of test compound or threshold dose that just inhibits growth:

	µg/ml
Brettanomyces anomolus	0.1
Pichia alcoholophilia	0.2
Endomycopsis javanensis	0.4
Hansenula saturnas	0.4
Rhodotorula sanniei	0.8
Schizosaccharomyces pombe	0.8
Candida pulcherrima	1.0
Torulaspora rosei	1.0
Cryptococcus neoformans	1.2
Candida albicans	1.2
Rhodotorula mucilaginosa	1.2
Saccharomyces ellipsoideus	1.6
Candida flereri	1.6
C. guilliermondi	1.6
Kloeckeria brevis	1.6
Histoplasma capsulatum (yeast phase on blood agar)	1.6
Saccharomycodes ludwigii	1.6
Saccharomyces cerevisiae	1.6
Helminthosporium sativum	1.6-3.2
Zygosaccharomyces mandshuricus	1.8
Endomyces magnusii	2.4
Rhizopus nigricans	3.2
Thamnidium elegans	3.2
Alternaria solani	3.2
Eremothecium ashbyii	3.2
Phycomyces blakesleeanus	3.2

(continued)

15. ASCOSIN (Concluded)

	μg/ml
Saccharomyces lactis	3.2
Candida krusei	3.2
Mycoderma cerevisiae	3.2
Penicillium spinulosum	3.2
Aspergillus niger	3.2
Debaromyces matruchoti	6.3
Candida monosa	6.4
C. tropicalis	8

[131]

In vivo. Some protection against Cryptococcus neoformans in mice. Prolonged survival time in mice infected with Histoplasma capsulatum. [121]

TOXICITY

Animal	Dose	mg/kg	Route	Reference
Mouse	LD_{50}	>500	p.o.	47
Mouse	LD_{50}	168	s.c.	47
Mouse	LD_{50}	8.6 ± 0.09	i.p.	47
Mouse	LD_0	10	i.v.	
Mouse	LD_{50}	12.5	i.v.	47
Mouse	LD_{100}	15.0	i.v.	

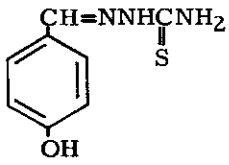
USE Medicinal.

16. BENZALDEHYDE, p-HYDROXY-, THIOSEMICARBAZONE

ALTERNATIVE NAME p-Hydroxybenzaldehyde thiosemicarbazone.

MOLECULAR FORMULA $C_8H_9N_3OS$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 195.242. Stable to heat.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm completely stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm did not inhibit spore germination. [55]

16. BENZALDEHYDE, p-HYDROXY-, THIOSEMICARBAZONE (Concluded)

TOXICITY 5 mice survived 500 mg/kg, i.p., daily for 7 days [260]. 500 mg/kg, s.t., non-lethal in rats [296].

USE Agricultural.

17. BENZENE, p-DICHLORO-

ALTERNATIVE NAMES PDB; p-Dichlorobenzene; 1,4-Dichlorobenzene.

MOLECULAR FORMULA $C_6H_4Cl_2$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES White crystals. Penetrating odor. [53] Molecular weight, 147.006. Melting point, 53°C. Boiling point, 173.7°C. Sublimes readily, leaving no residue. [53] Specific gravity, 1.4581 (20.5/4°C) [53,179]. Refractive index, 1.5518 (22°C) [192]. Soluble in alcohol, benzene, ether, chloroform, carbon disulfide. Insoluble in water. [53,118] Stable [179].

TOXICITY Man. Ingestion of 20 g has been well tolerated [101]. Continued exposure to vapors over a period of 1-2 years may cause hepatitis and cataract [192].

Animals. Irritation of mucous membranes, skin, cornea; liver and kidney damage [71]. Large doses cause liver injury and sometimes tremors [101]. LD_{50} in mice, 2950 mg/kg, p.o., in olive oil [47]. LD_{50} in rats, 2562 mg/kg, i.p. [120].

USE Agricultural: against tobacco blue mold [144].

CAUTION Use in well-ventilated area.

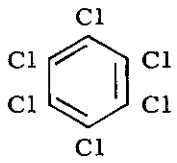
18. BENZENE, HEXACHLORO-

ALTERNATIVE NAMES Hexachlorobenzene; Perchlorobenzene.

MOLECULAR FORMULA C_6Cl_6

18. BENZENE, HEXACHLORO- (Concluded)

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [179], white to pale yellow [70], powder; white needles [53]. Molecular weight, 284.802. Melting point, 229°C. Boiling point, 326°C. [53] Vapor pressure, 1.089×10^{-5} mm Hg (20°C) [179]. Specific gravity, 2.044 (23°C) [118]. Soluble in benzene, boiling alcohol [46]. Insoluble in water [179].

TOXICITY Man. May cause irritation of the respiratory system, damage to the eyes; may have harmful effect on liver. [250] Very slight exfoliation with prolonged skin contact [101].

Animals. 500 mg/kg, i.p., non-lethal in rats [296]. Oral lethal dose in guinea pigs greater than 3 g/kg [101]. Toxic to fish, wildlife, and beneficial insects [289].

COMPARATIVE TOXICOLOGY Considered the least toxic of the chlorobenzenes [250].

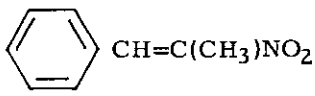
USE Agricultural: wheat bunt [95, 144].

19. BENZENE, (2-NITROPROPENYL)-

ALTERNATIVE NAME β-Methyl-β-nitrostyrene.

MOLECULAR FORMULA $C_9H_9NO_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 163.170.

TESTS In vitro. Activity against Trichophyton (gypseum) mentagrophytes as determined by the agar diffusion plate method:

Concentration, M	Inhibition Zone, cm
1×10^{-2}	Complete
5×10^{-3}	Complete
1×10^{-3}	Complete

(continued)

19. BENZENE, (2-NITROPROPENYL)- (Concluded)

Concentration, M	Inhibition Zone, cm
5×10^{-4}	Complete
1×10^{-4}	0.8
5×10^{-5}	1.0
1×10^{-5}	0.0
5×10^{-6}	0.0
1×10^{-6}	0.0

Fungi	Time of Exposure	mg/ml[1]					
		10	1	0.1	0.01	0.001	0.0001
Candida albicans	Immediate	-	-	+	+	+	+
	15 min	-	-	+	+	+	+
	30 min	-	-	+	+	+	+
Cryptococcus neoformans	Immediate	-	-	+	+	+	+
	15 min	-	-	-	+	+	+
	30 min	-	-	+	+	+	+
Trichophyton (gypseum) mentagrophytes	Immediate	-	-	-	+	+	+
	15 min	-	-	-	+	+	+
	30 min	-	-	-	+	+	+
Blastomyces dermatitidis	Immediate	-	-	-	-	+	+
	15 min	-	-	-	-	+	+
	30 min	-	-	-	-	-	+

[26]

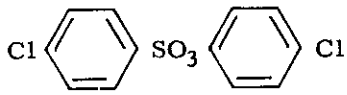
USE Medicinal.

20. BENZENESULFONIC ACID, p-CHLORO-, p-CHLOROPHENYL ESTER

ALTERNATIVE NAMES K6451; Orthotran; PCPCBS; p-Chlorophenyl-p-chlorobenzenesulfonate.

MOLECULAR FORMULA $C_{12}H_8Cl_2O_3S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White to tan, flaky solid. Molecular weight, 303.164. Melting point, approximately 80°C; 86.5°C (pure). Soluble in acetone, aromatic solvents. Moderately soluble in alcohol, petroleum oils. Practically insoluble in water. Hydrolyzed by alkalies. [180]

/1/ (-) = no growth on subculture; (+) = growth on subculture.

20. BENZENESULFONIC ACID, p-CHLORO-, p-CHLOROPHENYL ESTER (Concluded)

TOXICITY Man. Probable LD, 500-5000 mg/kg. Skin irritation, but no other symptoms, reported. [101]

Animals. Rats: LD_{50}, 2000 mg/kg, p.o. [120]. Diet containing 300 ppm for 130 days had no effect [180]. Liver and kidney damage with long exposure [101].

PHYTOTOXICITY Generally non-toxic to plants. Suspected injury to raspberry bushes [180].

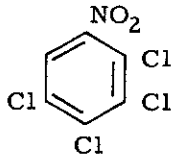
USE Agricultural.

21. BENZENE, 1,2,3,4-TETRACHLORO-5-NITRO-

ALTERNATIVE NAME 2,3,4,5-Tetrachloronitrobenzene.

MOLECULAR FORMULA $C_6HCl_4NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals. Molecular weight, 260.904. Melting point, 67°C. Soluble in alcohol. [29]

TESTS In vitro. 0.1 g of test compound deposited as a solid in the lid of a culture petri dish, reached test organism as a vapor. Radial growth of the colonies in culture plates was inhibited to a greater degree by the test compound than by a standard chemical, 2,3,5,6-tetrachloronitrobenzene, chosen for comparison.

	Growth Diameter, mm/da	% Inhibition
Fusarium caeruleum (Lib.) Sacc.		
Control	7.0	
2,3,5,6-Tetrachloronitrobenzene	4.5	36
Test compound	3.7	47
F. caeruleum, strain developed by McKee		
Control	5.3	
2,3,5,6-Tetrachloronitrobenzene	5.1	4
Test compound	3.7	30

[29]

21. BENZENE, 1,2,3,4-TETRACHLORO-5-NITRO- (Concluded)

PHYTOTOXICITY Potatoes, var. Craig's Defiance: 2 g of a 2% dust of the test compound, and of 2,3,5,6-tetrachloronitrobenzene, applied to 1-lb batches of tubers stored in closed tins until untreated controls were sprouting profusely. Test compound did not inhibit growth of sprouts.

	Mean Sprout Weights, g
Control	26.8
2,3,5,6-Tetrachloronitrobenzene	16.4
Test compound	27.9

[29]

Lettuce: Test compound as 5% dust, applied to leaves. Visible check to growth which was quickly overcome in the case of 2,3,5,6-tetrachloronitrobenzene, but which persisted in plants treated with test compound, producing significant reduction in dry weight of final crop. [29]

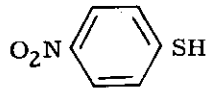
USE Protectant of materiel; agricultural.

22. BENZENETHIOL, p-NITRO-

ALTERNATIVE NAME p-Nitrothiophenol.

MOLECULAR FORMULA $C_6H_5NO_2S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 155.174. Insoluble in common solvents.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 100 μg/sq cm stopped spore germination. [55]

TOXICITY Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight. Inactive for 24 hours for all 3 species. [297].

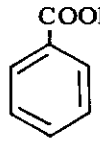
USE Agricultural; medicinal.

23. BENZOIC ACID

ALTERNATIVE NAMES Carboxybenzene; Phenylformic acid; Benzene carboxylic acid.

MOLECULAR FORMULA $C_7H_6O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [118], scales or needle-like crystals [222]; monoclinic tablets, plates, leaflets [192]. Molecular weight, 122.118. Melting point, 120-121°C [118]. Sublimes above 100°C [228]. Boiling point, 249°C [53]. Specific gravity, 1.2659 (15/4°C). Refractive index, 1.53974 (15°C). [118] Soluble in alcohol, ether, chloroform, benzene, acetone, carbon disulfide, carbon tetrachloride, turpentine. Slightly soluble in water [222].

TESTS In vitro. Aspergillus niger (Van Tiegham): 0.63% test compound in nutrient medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7); incubated 48 hours at 37°C. Inhibits growth. [181]

Epidermophyton floccosum (Harz) Langeron and Milochevitch, Cryptococcus neoformans, Microsporum felineum, Aspergillus fumigatus: Agar disks with organisms in solution of test compound. Washed 5 minutes; applied to Sabouraud's agar. 75,000 ppm abolished infestation. Same organisms on Sabouraud's agar plus horse serum, cap-plate method; incubated 3 weeks. 350 ppm abolished infestation. [165]

TOXICITY Man. Relatively non-toxic. Skin irritation with high concentrations. [273] Daily intake of 4-6 g caused no toxic symptoms aside from slight gastric irritation [105].

Animals. Large oral doses caused nausea and vomiting. Rats injected with compound exhibited tremors, convulsions, death. [101]

Animal	Dose	mg/kg	Route
Dog	LD	2000	p.o.
Guinea pig	LD	1400	i.p.
Rabbit	LD	2000[1]	p.o.
Rabbit	LD	2000[1]	s.c.
Rat	LD_{50}	1714 ± 124	i.v.
Frog	LD	100-200	s.c.

[120]

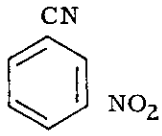
USE Protectant of materiel: paper, cotton textiles [111]. Agricultural: preservative for fats, fruit juices [192]. Medicinal: dermatomycoses [21, 222, 273]; combination of benzoic and salicyclic acids is one of the most useful antifungal preparations [73].

/1/ Approximately.

24. BENZONITRILE, m-NITRO-

MOLECULAR FORMULA $C_7H_4N_2O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow powder [100], needles [118]. Molecular weight, 148.118. Melting point, 115-116°C. Boiling point, 160-171°C (10 mm Hg). [100] Easily soluble in glacial acetic acid, ether, hot water, alcohol. Insoluble in petroleum ether [228].

TESTS In vitro. Nutrient-toxic-agar containing test compound, inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): 100% inhibition of growth at 250 and 100 ppm; 90% at 50 ppm. Trichoderma sp (USDA T-1): 100% inhibition of growth at 250 and 100 ppm. [100]

10-fold dilutions of compound added to spores in depression slide cavity. Stemphylium sarcinaeforme Cav.: MED, 10,000 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [100]

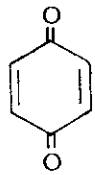
USE Protectant of materiel.

25. p-BENZOQUINONE

ALTERNATIVE NAMES Quinone; 1,4-Cyclohexadienedione; p-Quinone; 1,4-Quinone.

MOLECULAR FORMULA $C_6H_4O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow needles. Irritating odor. [53] Molecular weight, 108.092. Melting point, 115.7°C [53, 118]. Sublimes; volatile with steam, being in part decomposed. [53] Specific gravity, 1.307 [53], 1.318 [118]. Soluble in alcohol, hot ligroin, alkalies, ether. Slightly soluble in water. [118] Stable.

25. p-BENZOQUINONE (Concluded)

TESTS In vitro. Alternaria oleracea Milb., and Sclerotinia fructicola (Wint.) Rehm.: Test tube dilution technique, as recommended by the Council of the American Phytopathological Society; glass slide, spore germination inhibition test. ED_{50}, 0.01-0.1 ppm concentration. [189]

Aspergillus niger: Nutrient medium, 37°C; 48 hours evaluation time. Growth of inoculum inhibited; MED, 0.13%. [189]

In vivo. Alternaria solani (Ell. and Mart.) J. and G.: 2000 ppm slightly effective in control of foliage infection in tomato plants. [189]

TOXICITY Man. Probable LD, 50-500 mg/kg. Has produced ocular and cutaneous lesions in man, but no systemic poisonings reported. [101]

Animals. LD_{50} in rats, approximately 130 mg/kg, p.o.; 25 mg/kg, i.v. [120].

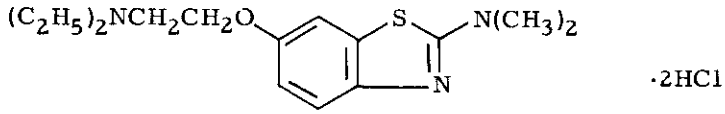
PHYTOTOXICITY Not significantly toxic to plants [138].

USE Protectant of materiel; agricultural.

26. BENZOTHIAZOLE, 6-(2-DIETHYLAMINOETHOXY)-2-DIMETHYLAMINO-, DIHYDROCHLORIDE

ALTERNATIVE NAMES Dihydrochloride of 2-dimethylamino-6-(β-diethylaminoethoxy)-benzothiazole [281]; 6-(β-Diethylaminoethoxy)-2-dimethylamino-benzothiazole dihydrochloride [191]; Diamthazole dihydrochloride; Asterol dihydrochloride.

MOLECULAR FORMULA $C_{15}H_{23}N_3OS \cdot 2HCl$

STRUCTURAL FORMULA 

PHYSICAL AND CHEMICAL PROPERTIES Colorless [273], crystals [192]. Molecular weight, 366.354. Decomposes, 269°C. Freely soluble in water, methanol, ethanol. A 5% aqueous solution has a pH of approximately 2 [192].

TESTS In vitro. Susceptible organisms: Candida albicans, Epidermophyton floccosum, Microsporum audouini, M. canis, M. gypseum, Trichophyton (gypseum) mentagrophytes, T. (purpureum) rubrum, T. (Achorion) schoenleinii, T. tonsurans, T. violaceum [222].

26. BENZOTHIAZOLE, 6-(2-DIETHYLAMINOETHOXY)-2-DIMETHYLAMINO-, DIHYDROCHLORIDE (Concluded)

TOXICITY Man. Skin irritation negligible in concentrations of 2-5%. May produce hallucinations, convulsions in children. Not recommended for infants under 2 years. [273] Reported to cause encephalopathy in children under 5 years. Not to be used in acute stage of dermatomycoses. [222] Convulsions may result from prolonged use of ointment on scalps of young children with tinea capitis, otherwise toxicity is very low and sensitization is negligible. [73]

Animals. LD_{50} in mice, 0.5 g/kg, p.o.; 0.375 g/kg, s.c. [47]

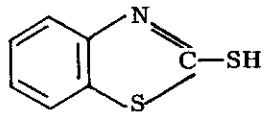
USE Medicinal: Potent agent in treatment of ringworm of the scalp, tinea versicolor, and infections of skin and nails caused by Candida albicans; also in treatment of athlete's foot and ringworm on inside of thighs; superficial fungus infections. [21, 31, 73, 201]

27. BENZOTHIAZOLE, 2-MERCAPTO-

ALTERNATIVE NAMES o-Thiocarbamidothiophenol; MBT; 2-Benzothiazolethiol; 2-Mercaptobenzothiazole.

MOLECULAR FORMULA $C_7H_5NS_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White needles or leaflets [318]; yellowish powder [53]. Slight odor [53]. Molecular weight, 167.250. Melting point, 179°C [318], 179.5°C [118], 170-175°C [252], 169-176°C [228]. Specific gravity, 1.42 [252]. Soluble (g/100 g solvent at 25°C) in water, <0.005; acetone, 19.7; acetic acid, 0.61; benzene, 0.52; chloroform, 1.2; diethyl ether, 3.62; ethanol, 5.2; n-heptane, <0.02; mineral oil, <0.02; toluene, 0.43. [229] Soluble in hot alcohol [118].

TESTS In vitro. Aspergillus niger (Van Tiegham): 250 ppm gave 100% inhibition. LD_{50}, 32 ppm. [228]

A. niger (Van Tiegham):

x 10^{-4} M	6	5	4	3	2	1
% inhibition	100	100	100	89	72	14

[228]

Sterigmatocystis nigra, and Penicillium notatum: Growth inhibited by 0.0005 M. [174].

27. BENZOTHIAZOLE, 2-MERCAPTO- (Concluded)

Samples of No. 8 cotton duck sprayed with 1% solution inhibited growth of mildew organisms, in a moist, warm atmosphere, for 60 days [174].

TOXICITY Man. Possible skin absorption with prolonged contact [174].

Animals. Leather preserved with 0.25-0.50% of compound found safe to use on dogs and horses [174].

PHYTOTOXICITY Not significantly toxic to plants [138].

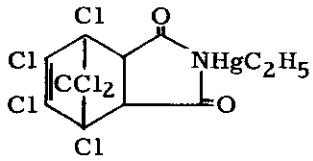
USE Protectant of materiel: textiles, leather [227]. Medicinal: superficial mycoses [252].

28. BICYCLO [2, 2, 1] HEPT-5-ENE-2, 3-DICARBOXIMIDE, 1, 4, 5, 6, 7, 7-HEXACHLORO-N-(ETHYLMERCURI)-

ALTERNATIVE NAMES N-Ethylmercuri-1, 2, 3, 6-tetrahydro-3, 6-endomethano-3, 4, 5, 6, 7, 7-hexachlorophthalimide; 1, 4, 5, 6, 7, 7-Hexachloro-N-(ethylmercuri) bicyclo [2, 2, 1] hept-5-ene-2, 3-dicarboximide.

MOLECULAR FORMULA $C_{11}H_7Cl_6HgNO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals. Molecular weight, 598.526. Melting point, 190-192°C. Soluble in acetone and other ketones at room temperature. Moderately soluble in alcohol. Slightly soluble in hydrocarbons. Insoluble in water. Relatively stable in heat, light, moisture. With prolonged weathering, compound breaks down to water solution products. [179]

PHYTOTOXICITY Injurious to rose plants [179].

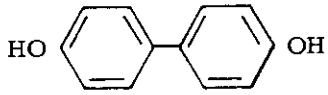
USE Agricultural: Powerful inhibitor of fungus spore germination [179].

29. p,p'-BIPHENOL

ALTERNATIVE NAME 4,4'-Dihydroxybiphenyl.

MOLECULAR FORMULA $C_{12}H_{10}O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Rhombic needles or plates [118]. Molecular weight, 186.200. Melting point, 269-272°C [53], 274-275°C [118]. Soluble in alcohol, ether. Slightly soluble in water, benzene. [52,118]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 84% inhibition of growth at 250 ppm; 100% inhibition of growth at 250 ppm. [52]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm. [52]

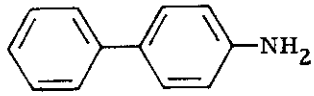
USE Protectant of materiel.

30. 4-BIPHENYLAMINE

ALTERNATIVE NAMES 4-Aminodiphenyl; Xenylamine.

MOLECULAR FORMULA $C_{12}H_{11}N$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless to grayish crystals. Molecular weight, 169.216. Melting point, 53°C. Boiling point, 302°C. Specific gravity, 1.160 (20/20°C). [118] Soluble in alcohol, ether [46]; chloroform, methanol [118]. Slightly soluble in water [53].

30. 4-BIPHENYLAMINE (Concluded)

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm completely stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 100 μg/sq cm completely stopped spore germination. [55]

TOXICITY Man. Probable LD, 500-5000 mg/kg [101].

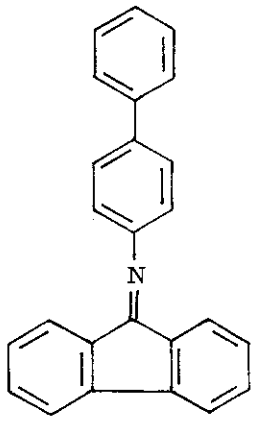
Animals. When given by mouth (in oil solution) to laboratory animals, compound caused anorexia, diarrhea, emaciation, hypothermia, and general debility; in cats, methemoglobinemia. [101] MTD in mice (Banks, adult males), 125 mg/kg, i.p., in isotonic saline solution. LD_{50} in rats, approximately 500 mg/kg, s.t., in propylene glycol. [260]

USE Agricultural.

31. 4-BIPHENYLAMINE, N-9-FLUORENYLIDENE-

MOLECULAR FORMULA $C_{25}H_{17}N$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 331.394. Melting point, 191-192.5°C. Soluble in alcohol. Slightly soluble in petroleum ether. Possibly light sensitive; sensitive to acids.

TESTS In vitro. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 1 μg/sq cm completely stopped spore germination [55].

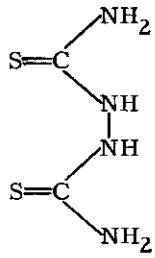
USE Agricultural.

32. BIUREA, 2,5-DITHIO-

ALTERNATIVE NAMES Bisthio-carbamyl hydrazine; Bis(thiourea).

MOLECULAR FORMULA $C_2H_6N_4S_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystalline solid. Molecular weight, 150.232. Decomposes, 221-223°C. Very slightly soluble in cold water. Insoluble in alcohol.

TESTS In vitro. 1000 µg/sq cm inhibited spore germination: Sclerotinia fructicola (Wint.) Rehm., 100%; Stemphylium sarcinaeforme Cav., 53%. [55]

Actinomyces bovis, 3 strains, 2 human and 1 bovine: In thioglycollate broth; 200 µg/ml incubated 10 days at 37°C. No inhibition of growth. [271]

Nocardia asteroides, 10 strains; 1 strain each of N. mexicanus, N. madurae, N. purpureum, N. hemolyticus: On Sabouraud's agar; incubated 6-8 days at 37°C. 10-50 µg/ml gave partial inhibition; 10->200 µg/ml completely inhibited growth. [271]

In vivo. Not effective in mice against Cryptococcus hominis, Blastomyces dermatitidis, Nocardia asteroides [271].

TOXICITY Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 6 ppm by weight; exposure 24 hours. No injury. [297]

USE Medicinal.

33. BORAX

ALTERNATIVE NAMES Sodium tetraborate; Sodium borate; Sodium biborate.

MOLECULAR FORMULA $B_4Na_2O_7 \cdot 10H_2O$

33. BORAX (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Colorless [118], or white [180], monoclinic [118], crystals [228]. Molecular weight, 381.434. Melting point, 75°C. Specific gravity, 1.73. Refractive index, 1.447, 1.469, 1.472. Soluble in water (g/100 ml), 1.3 at 0°C, 1.6 at 10°C, 14.2 at 55°C. Soluble in glycerin. Very slightly soluble in alcohol. Insoluble in acid. [118]

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 8% solution of test compound, dried, and stored for 3 weeks at 70°F. Decay prevented; no rind injury. [291]

TOXICITY Man. Low. Probable LD, 0.5-5 g/kg [101]; 5-15 g/kg [71]. Skin excoriations, fever, and anuria [71].

PHYTOTOXICITY Highly toxic to plants [180].

USE Protectant of materiel: leather, paint, adhesives, wood [53, 111]. Agricultural: citrus mold preventive [180].

34. BORDEAUX MIXTURE[1]

REACTANTS Copper sulfate; Calcium hydroxide.

PHYSICAL AND CHEMICAL PROPERTIES Flocculent blue liquid; slowly settling amorphous precipitate becomes crystalline. [179] Almost insoluble in water. Unstable with metals. [56]

TOXICITY Man. Probable LD 50-500 mg/kg [101]. Irritating to nose and throat. Absorption generally poor. [56]

PHYTOTOXICITY May cause injury to certain trees and plants, such as apple, peach, raspberry, cantaloupe, cucumber, and watermelon [56, 144].

COMPARATIVE TOXICOLOGY Less astringent and presumably less toxic than copper sulfate [101].

USE Agricultural: general-purpose fungicide for foliage application [125, 179].

/1/ Slaked lime plus copper sulfate.

35. BORIC ACID

ALTERNATIVE NAMES Boracic acid; Orthoboric acid.

MOLECULAR FORMULA BH_3O_3

PHYSICAL AND CHEMICAL PROPERTIES Colorless scales or white powder. Odorless. [53] Molecular weight, 61.844. Melting point, 184°C [53]. Specific gravity, 1.4347 [53], 1.435 (15/4°C) [118]. Refractive index, 1.340 [118]. Soluble in water, alcohol, glycerin [53]. Slightly soluble in acetone [118]. Stable in air [53]. Acid to litmus [35].

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges, dipped in 5% of test compound, dried, and stored 3 weeks at 70°F. Decay prevented; no rind injury. [291, 293]

TOXICITY Man. Probable LD, 15-20 g in adults, 5-6 g in infants. Relatively large amounts are localized in the brain, liver and kidneys. Large doses produce nausea, vomiting, diarrhea; body temperature falls and erythematous rash similar to scarlet fever develops; followed by desquamation. Headache, restlessness, weakness. Renal injury often occurs. Death from circulatory collapse and shock usually within 5 days. [105, 154]

Animals. Experimental animals show no deleterious effects from daily ingestion of moderate amounts. [105]

Animal	LD_{50}, mg/kg	Route
Dog	>1000	p.o.
Guinea pig	1200 ± 80	s.c.
Mouse	3450 ± 158	p.o.
Mouse	1740 ± 130	s.c.
Mouse	2070 ± 170	s.c.
Mouse	1780 ± 121	i.v.
Rat	5140(4740-5580)	p.o.
Rat	2660 ± 220	p.o.
Rat	1330 ± 112	i.v.

[120]

USE Protectant of materiel: leather [53]. Agricultural: food preservative [99, 105]. Medicinal.

36. BUTYL PHOSPHITE, DI-, SODIUM SALT

ALTERNATIVE NAME Sodium dibutyl phosphite.

MOLECULAR FORMULA $C_8H_{18}O_3P{\cdot}Na$

STRUCTURAL FORMULA $[CH_3(CH_2)_3O]_2PONa$

PHYSICAL AND CHEMICAL PROPERTIES Colorless, liquid grease. Molecular weight, 216.196. Boiling point, 110-111°C (6 mm Hg), 118-119°C (7 mm Hg). Specific gravity, 0.987. Refractive index, 1.4238, 1.4222 (27°C). Soluble in hexane, water (hydrolyzes very rapidly), most organic solvents.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1 μg/sq cm completely stopped spore germination [55].

Sclerotinia fructicola (Wint.) Rehm.:

Concentration μg/sq cm	% Inhibition
1000	100
100	77
10	0
1	0

[55]

TOXICITY Mice, adult females: Compound, in butyl succinate solution, administered i.p. daily for 5 days. 250 cu mm/kg, no chronic toxic effects; 500 cu mm/kg, chronic effects. [260]

USE Agricultural.

37. BUTYRIC ACID, 3,3-DIMETHYL-

ALTERNATIVE NAMES Pentiformic acid; Caproic acid; Capronic acid; Hexanoic acid; tert.-Butylacetic acid; Pentylformic acid; Hexylic acid; Hexoic acid.

MOLECULAR FORMULA $C_6H_{12}O_2$

STRUCTURAL FORMULA $(CH_3)_3CCH_2COOH$

PHYSICAL AND CHEMICAL PROPERTIES Colorless or slightly yellow liquid. Odor like that of limburger cheese. Molecular weight, 116.156. Freezing point, -5.4°C. Boiling point, 205°C. Specific gravity, 0.9295 (20/20°C). Refractive index, 1.4164. Soluble in alcohol, ether. Slightly soluble in water. [53]

37. BUTYRIC ACID, 3,3-DIMETHYL- (Concluded)

TESTS In vitro. Trichophyton (gypseum) mentagrophytes, strain 640: Conidia seeded on agar plate, incubated at 30°C; undiluted test compound. Decreased infestation by 4.5 cm (radius of inhibited zone). [210]

TOXICITY May cause opaque cornea, keratoconus, and necrosis of the cornea in man [250].

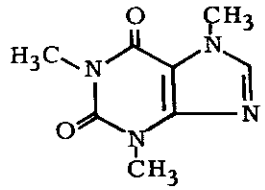
USE Medicinal.

CAUTION Handlers should wear chemical safety goggles. Moderate fire hazard. [250]

38. CAFFEINE

MOLECULAR FORMULA $C_8H_{10}N_4O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 194.192. Melting point, 235-237°C. Soluble in hot water, hot alcohol, chloroform, ethyl acetate. [228]

TESTS In vitro. Ophiostoma multiannulatum: Conidia and test compound in nutrient medium[1]. 0.05-0.15% caused decrease in multiplication rate. No growth at 0.2%. 0.2% caused biochemical mutations. [97]

TOXICITY Man. LD in adults probably exceeds 10 g [97]. Restlessness, excitement, tinnitus; rapid pulse and extrasystole often evident. [101] Nausea, vomiting, insomnia, convulsions [190].

/1/ Method of Fries (Physiologia Plantarum 1:330, 1948).

38. CAFFEINE (Concluded)

Animals.

Animal	Dose	mg/kg	Route	Time of Death	Reference
Cat	MLD	100-150	p.o.		120
Cat	MLD	150	s.c.		120
Cat	MLD	180-200	i.p.		120
Cat	MLD	80-100	i.v.		120
Cat	LD	150-155	s.c.	1 hr ±	120
Cat	LD	175	i.v.		120
Dog	MLD	140-150	p.o.		120
Dog	MLD	500	s.c.		120
Dog	LD_{50}	175	i.v.		120
Dog	LD	110	s.c.	Few hr	120
Guinea pig	MLD	200-240	s.c.		120
Guinea pig	MLD	220-250	i.p.		120
Mouse	MLD	220	i.p.		120
Mouse	LD_{50}	615-735	s.t.		218
Mouse	LD_{50}	100.9 ± 6.67	i.v.		120
Mouse	LD	180-190	s.c.	2-3 da	120
Mouse	LD	250	i.p.		120
Mouse	LD	500	i.p.		120
Mouse	LD	500	i.p.	8 min	266
Rabbit	MLD	290-350	p.o.		120
Rabbit	MLD	200-300	s.c.		120
Rabbit	LD	350-360	p.o.		120
Rabbit	LD	270-280	s.c.	1-4 hr	120
Rabbit	LD	200	i.m.	4 hr	120
Rabbit	LD	80-100	i.v.		120
Rat	MLD	210-280	i.p.		120
Rat	LD_{50}	200	p.o.		120
Rat	LD_{50}	233 ± 14	p.o.		120
Rat	LD_{50}	104.8 ± 1.87	i.v.		120
Rat	LD	70-130	s.c.		120
Rat	LD	250	s.c.	2 hr	120
Frog	LD	120-130	s.c.	4-5 da	120

USE Protectant of materiel.

39. CANDICIDINS A, B, C

SOURCE Streptomyces griseus and other Streptomyces spp [121].

PHYSICAL AND CHEMICAL PROPERTIES Soluble in higher alcohols. Insoluble in benzene, petroleum ether, carbon tetrachloride, xylene, carbon disulfide, ethylene dichloride, ether, ethyl acetate. Only Candicidin A is soluble in water. Concentrated

39. CANDICIDINS A, B, C (Concluded)

solutions more stable than dilute. A and B stable at neutrality for 10 minutes at 60°C, and for one week at 4°C. Activity gradually lost at room temperature. [121]

TESTS In vitro. Candicidin A and B inhibit, at 0.5-10 μg/ml, Candida albicans, C. stellatoidea, C. tropicalis, C. pseudotropicalis, C. krusei, Blastomyces dermatitidis, Histoplasma capsulatum, Paracoccidioides brasiliensis, Cryptococcus neoformans, Geotrichum spp, Hormodendrum pedrosoi. Candida parakrusei inhibited at 25-50 μg/ml. Less sensitive, 200-500 μg/ml: Coccidioides immitis, Sporotrichum schenckii, Nocardia asteroides, Trichophyton spp, Microsporum canis, M. audouini, Epidermophyton floccosum. Candicidin C is relatively inactive. [121]

In vivo. Candicidin A and B protected mice against infections with Candida albicans, Blastomyces dermatitidis, Sporotrichum schenckii. Little or no activity against Coccidioides immitis and Histoplasma capsulatum following i.p. doses of 37.5 mg/kg/da for 10 days. [121]

Crude preparations decreased powdery mildew in young bean plants sprayed once weekly with 660 μg/ml solution. Concentration of 1:16,000 was excellent protective dip against brown rot of peach fruit. Failed to control effectively stem rust of wheat when used as a preinoculation spray under greenhouse conditions. [121]

TOXICITY Candicidin A: LD_{50} in mice, 277 mg/kg, s.c.; 47-65 mg/kg, i.p. Candicidin B: LD_{50} in mice, 159 mg/kg, s.c.; 53 mg/kg, i.p. Necrosis developed at site of injection of 25 mg/kg, s.c. [121]

PHYTOTOXICITY No toxic effect on bean plants at 660 μg/ml or on germination of pea seeds at 125 μg/ml [121].

USE Medicinal; agricultural.

40. CANDIDINS A, B

SOURCE Streptomyces viridoflavus [53,121].

PHYSICAL AND CHEMICAL PROPERTIES Soluble at neutral and alkaline pH. Free acid: soluble in ethanol, methanol, glacial acetic acid, ethylene glycol monomethyl ether, pyridine, other basic solvents. Free acid (Na salt): insoluble, or slightly soluble, in ether, chloroform, acetone, benzene, non-polar solvents. Separated by solvent extraction into 2 fractions, A and B, but A is probably an artifact. [121]

TESTS In vitro. Candida albicans, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, Blastomyces dermatitidis, and Sporotrichum schenckii inhibited at 0.2-41 μg/ml [121].

40. CANDIDINS A, B (Concluded)

In vivo. Candidin B: Daily oral doses of 100μg/kg resulted in complete suppression of fungi, with a concomitant 1000-fold increase in bacterial fecal flora of mice [121].

TOXICITY Animals. Crude preparations: LD_{50} in mice, 7-36 mg/kg, i.p. Candidin B: LD_{50} in mice, 1.5 mg/kg, i.v.; 30 mg/kg, s.c., with necrosis at site of injection after single doses of 10-40 mg/kg. [121,274]

Daily oral doses of 100 mg/kg for 6 days well tolerated in mice, but spleen showed reduction in size [121].

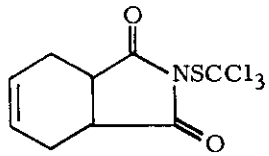
USE Medicinal.

41. CAPTAN

ALTERNATIVE NAMES N-Trichloromethylmercapto-4-cyclohexene-1,2-dicarboximide; N-Trichloromethylthio-tetrahydrophthalimide.

MOLECULAR FORMULA $C_9H_8Cl_3NO_2S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White to cream-colored powder (pure) [53], yellow amorphous powder (tech.) [318]. Slight odor (pure); pungent (tech.). [318] Molecular weight, 300.599. Melting point, 172-173°C (pure), 158-164°C (tech.). [318] Specific gravity, 1.5. Partially soluble in acetone, benzene, toluene. Slightly soluble in ethylene dichloride, chloroform. [53] Practically insoluble in water. Stable under alkaline conditions. [180]

TESTS In vitro. Stemphylium sarcinaeforme Cav. spores: LD_{50}, 3.6 μg/sq cm [138].

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	77

x 10^{-5} M	7.5	5.0	2.5	1.0
% inhibition	61	57	52	37

250 ppm inhibited growth 100%. [228]

41. CAPTAN (Concluded)

TOXICITY Man. May cause skin irritation [95]. No poisonings reported [101].

Animals. Low toxicity in laboratory and farm animals [101]. Rats: LD_{50}, 15,000 mg/kg, p.o.; 50-100 mg/kg, i.p. [120]

PHYTOTOXICITY No evidence of toxicity in plants [180]. Sometimes produces "frog-eye" leaf spot on apple foliage [138].

USE Protectant of materiel: paints, plastics, leather, fabrics [53]. Agricultural: widely used around the world as an agricultural spray [138]; seed treatment [53].

CAUTION Avoid inhalation of dust or spray, prolonged or repeated skin contact [53].

42. CARBAMIC ACID, DIETHYLDITHIO-, COPPER (II) SALT

ALTERNATIVE NAME Copper diethyl dithiocarbamate.

MOLECULAR FORMULA $C_{10}H_{20}N_2S_4 \cdot Cu$

STRUCTURAL FORMULA $[(C_2H_5)_2NCSS]_2Cu$

PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 360.080. Very soluble in chloroform, carbon disulfide. Soluble in benzene, acetone. Slightly soluble in alkalies, ether.

TESTS In vitro. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 1000 µg/sq cm completely stopped spore germination [55].

TOXICITY Laboratory rats (albino and hooded, weighing 130-200 g): Test compound dissolved in 2% gum acacia. MLD, 250 mg/kg, i.p.; >1000 mg/kg, s.t., non-toxic.

USE Agricultural.

43. CARBAMIC ACID, DIETHYLDITHIO-, MERCURY (II) SALT

ALTERNATIVE NAME Mercuric diethyl dithiocarbamate.

MOLECULAR FORMULA $C_{10}H_{20}N_2S_4 \cdot Hg$

STRUCTURAL FORMULA $(C_2H_5)_2NCSS\rangle Hg$
$(C_2H_5)_2NCSS\rangle$

43. CARBAMIC ACID, DIETHYLDITHIO-, MERCURY (II) SALT (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White powder. Molecular weight, 497.150. Melting point, 115-119°C. Soluble in acetone, carbon disulfide, benzene. Very soluble in chloroform. Slightly soluble in alcohol, ether.

TESTS In vitro. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 1 μg/sq cm completely stopped spore germination [55].

TOXICITY Rats (albino and hooded): MLD, 100 mg/kg, i.p.; >1000 mg/kg, s.t., non-toxic. [213, 296]

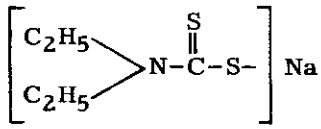
USE Agricultural.

44. CARBAMIC ACID, DIETHYLDITHIO-, SODIUM SALT

ALTERNATIVE NAME Sodium diethyldithiocarbamate.

MOLECULAR FORMULA $C_5H_{11}NS_2 \cdot Na$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White or colorless crystals [53]. Molecular weight, 171.267. Soluble in water, hot alcohol. Stable in dry state.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm completely stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 100 μg/sq cm completely stopped spore germination. [53]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, Epidermophyton floccosum (Harz) Langeron and Milochevitch, and Sporotrichum schenckii: Sabouraud's agar (Difco) streaked with 10-day growth of test organism from agar slant. Test compound in 50 ppm concentration (incubated for 15 days at 25°C) did not completely inhibit growth. [38]

In vivo. Apple tree, var. "Delicious": 27 years old, in leaf; tested for spray injury and development of anthocyanin fruit pigments. 3 bearing limbs of tree selected and given thorough spray application; 2 limbs received similar application after 1 week, and 1 limb a third application, 1 week later. Rest of tree served as control. 5,000 and 10,000 ppm used. First application gave moderate leaf injury; second and third gave moderate to considerable foliage injury. Test compound combined with 2,4,5-trichlorophenoxy acetic acid gave synergistic effect on anthocyanin fruit-developing pigments at 2500 ppm, with first and second applications producing only slight foliage injury, and moderate injury after third spray application. [321]

44. CARBAMIC ACID, DIETHYLDITHIO-, SODIUM SALT (Concluded)

TOXICITY Man. Skin irritant [250].

Animals. Mice: 500 mg/kg of test compound, i.p. daily for 5 days, did not produce death (MTD). [260]

USE Medicinal. Agricultural. Protectant of materiel: fungus-proofing of textiles [250].

45. CARBAMIC ACID, DIMETHYLDITHIO-, IRON SALT

ALTERNATIVE NAMES Ferbam; Ferric dimethyldithiocarbamate.

MOLECULAR FORMULA $C_9H_{18}FeN_3S_6$

STRUCTURAL FORMULA $[(CH_3)_2NCSS]_3Fe$

PHYSICAL AND CHEMICAL PROPERTIES Black or dark-colored, fluffy powder [53]. Molecular weight, 416.504. Decomposes above 180°C [53, 180]. Vapor pressure negligible at 25°C [180]. Soluble in chloroform, acetone, pyridine, acetonitrile [129, 180]. Very slightly soluble in water [53]. Stable; some tendency to decompose with prolonged storage or exposure to moisture or heat [180]. pH of saturated solution, 5.0 [53].

TOXICITY Man. Probable LD, 500-5000 mg/kg [101]. Irritating to eyes, nose, throat, skin [53]. Kidney damage reported [101].

Animals. No effect on weanling rats fed 0.01% in diet for 30 days. Dogs tolerated 25 mg/kg fed daily for 1 month. Toxic effects apparent when treatment lasted 1 year; none at 5 mg/kg level. [180] 2-year dietary feeding to rats: 0.25% affected growth and mortality; no toxic effects from 0.025%. [171]

Animal	LD_{50}, mg/kg	Route	Reference
Guinea pig, ♂	450-2000	i.p.	120
Mouse, ♂	3000 ± 230	i.p.	120
Mouse	315[1]	i.p.	47
Rabbit, ♂	2000-3000	i.p.	120
Rat	4000	p.o.	180
Rat, ♂	2700 ± 96	i.p.	120
Rat, ♀	>17,000	i.p.	120

/1/ In 10% gum acacia suspension.

45. CARBAMIC ACID, DIMETHYLDITHIO-, IRON SALT (Concluded)

PHYTOTOXICITY Relatively non-toxic to plants [95, 144].

USE Agricultural: fruit crops and ornamentals [180].

CAUTION Avoid use with copper or mercury compounds. Incompatible with lime. [53]

46. CARBAMIC ACID, DIMETHYLDITHIO-, SODIUM SALT

ALTERNATIVE NAMES Sodium dimethyldithiocarbamate; Dimethyldithiocarbamic acid, sodium salt.

MOLECULAR FORMULA $C_3H_6NS_2 \cdot Na$

STRUCTURAL FORMULA $(CH_3)_2NCSSNa$

PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 143.215. Soluble in alcohol, acetone, water. Stable in dry state.

TESTS In vitro. Penicillium italicum (Wehmer): 10 ppm completely inhibited spore germination (approximately 5×10^3 spores/ml), at pH 6.8; minimum fungistatic concentration, 0.2 ppm. [147]

TOXICITY Man. Skin irritant [250].

Animals. LD_{50} in mice, 560 mg/kg, i.p. [170].

PHYTOTOXICITY Not significant [138].

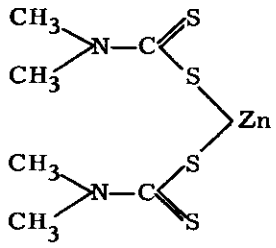
USE Protectant of materiel: textiles [227]. Also agricultural.

47. CARBAMIC ACID, DIMETHYLDITHIO-, ZINC SALT

ALTERNATIVE NAMES Ziram; Zinc dimethyl dithiocarbamate.

MOLECULAR FORMULA $C_6H_{12}N_2S_4Zn$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White powder or solid [118, 180]. Odorless when pure. Molecular weight, 305.816. Melting point, 246°C (pure), 240-244°C (tech.) [53, 318]; 240°C [180], 248-250°C [118]. Specific gravity, 2.00 [118]. Soluble (g/100 g solvent at 25°C) in water, <0.008; acetic acid, <0.02; acetone, 0.33; benzene, 0.06; chloroform, 0.74; diethyl ether, <0.02; ethanol, <0.03; n-heptane, <0.006; mineral oil, <0.01; toluene, <0.01. Soluble (1%) in dibutyl phthalate, tributyl phosphate, methyl phthallyl glycollate. Soluble (g/100 ml), dimethyl formamide, 3.75; ethylene dichloride, 0.9; methyl ethyl ketone, 0.5. Soluble in carbon disulfide, dilute alkalies, strong ammonia solution. [318] Unstable to ultraviolet light, high temperatures, acidic conditions.

TESTS In vitro. Stemphylium sarcinaeforme Cav. spores: LD_{50}, 0.51 µg/sq cm of sprayed surface [138].

TOXICITY Man. Probable LD, 50-500 mg/kg [101]. Irritating to skin and mucous membranes in dust or vapor form [53, 95, 101, 180]. Metallic taste in mouth, pains, purging, collapse [190].

Animals. Toxic in guinea pigs and rabbits, less so in rats [101].

Animal	LD_{50}, mg/kg	Route
Guinea pig	100-150	p.o.
Guinea pig	20-30	i.p.
Mouse	73 ± 11	i.p.
Rabbit	100-1020	p.o.
Rabbit	400	p.o.
Rabbit	5-50	i.p.
Rat	1400 ± 99	p.o.
Rat	23 ± 2	i.p.
Rat	33 ± 5	i.p.

[96, 134]

PHYTOTOXICITY Relatively non-toxic to plants [95].

COMPARATIVE TOXICOLOGY Action similar to that of ferbam (carbamic acid, dimethyldithio-, iron salt) [96].

USE Protectant of materiel: fabrics[1], paper, leather [125]. Agricultural: fruit and vegetable crops [180].

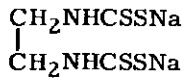
/1/ Approved by Surgeon General in concentrations up to 1% in fabrics [300, 301].

48. CARBAMIC ACID, ETHYLENEBIS(DITHIO-, DISODIUM SALT

ALTERNATIVE NAMES Nabam; Disodium ethylenebisdithiocarbamate.

MOLECULAR FORMULA $C_4H_6N_2Na_2S_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Dark yellow [144], colorless (pure), crystals. Sulfur-like odor. Molecular weight, 256.362. Vapor pressure negligible at 25°C. Easily soluble in water. [53] Unstable to heat, light, moisture [129].

TOXICITY Man. Probable LD, 500-5000 mg/kg [101]. Mild skin irritation. Compound has goitrogenic and sensitizing properties. [56] Patch testing developed sensitization reactions in half of subjects tested [171].

Animals. CNS depression, mild skin irritation [101]. Goitrogenic in rats [149]. Weanling rats on diet containing 0.1% or more of compound showed greatly increased thyroid weight and epithelial hyperplasia [171]. LD_{50} in rats, approximately 395 mg/kg [47, 120, 149].

PHYTOTOXICITY Highly toxic to plant foliage [179].

COMPARATIVE TOXICOLOGY About 10 times as toxic as zineb (carbamic acid, ethylenebis [dithio-, zinc salt) [149].

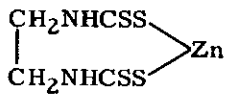
USE Agricultural: protective fungicide for vegetables, ornamentals, tobacco [56].

49. CARBAMIC ACID, ETHYLENEBIS(DITHIO-, ZINC SALT

ALTERNATIVE NAMES Zineb; Zinc ethylenebisdithiocarbamate.

MOLECULAR FORMULA $C_4H_6N_2S_4Zn$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light [53, 179], white to off-white [129], solid [53], powder [179]. Molecular weight, 275.748. Vapor pressure negligible at 25°C [179]. Insoluble in water [53, 179]. Unstable to light, heat, moisture. May polymerize. [179]

TOXICITY Man. Probable LD, 5-15 g/kg [101]. May cause irritation to mucous membranes and skin [95, 101, 179]. Goitrogenic properties [56].

49. CARBAMIC ACID, ETHYLENEBIS(DITHIO-, ZINC SALT (Concluded)

Animals. LD_{50} in rats, >5200 mg/kg, p.o. [47, 56, 120, 149]. One-year feeding in diet to dogs showed that 1% had no effect on growth, blood, mortality; some evidence of thyroid enlargement. Two-year feeding in diet to rats showed that 1% diminished growth; 0.1% and above produced hyperplasia of the thyroid. [171]

PHYTOTOXICITY Relatively non-toxic to plants [95].

COMPARATIVE TOXICOLOGY Toxic action similar to that of ferbam (carbamic acid, dimethyldithio-, iron salt) [96]. About one-tenth as toxic as nabam (carbamic acid, ethylenebis [dithio-, disodium salt) [149].

USE Agricultural: protective fungicide for foliage [179].

CAUTION Keep away from fire.

50. CARBAMIC ACID, METHYLDITHIO-, SODIUM SALT

ALTERNATIVE NAMES Sodium N-methyl dithiocarbamate dihydrate; Sodium methyl dithiocarbamate.

MOLECULAR FORMULA $C_2H_4NNaS_2$

STRUCTURAL FORMULA $CH_3NHCSSNa$

PHYSICAL AND CHEMICAL PROPERTIES White crystals [249]. Molecular weight, 129.189. Soluble in water. Moderately soluble in alcohol. Stable in concentrated aqueous solution, but decomposes in dilute aqueous solution.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 100 μg/sq cm completely stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 10 μg/sq cm completely stopped spore germination. [55]

100 ppm on unsealed agar plates gave 100% kill of the following: Phytophthora cactorum, P. cinnamoni, P. citrophthora, Pythium aphanidermatum, P. ultimum, Rhizoctonia solani, Sclerotinia sclerotiorum, Sclerotium rolfsii [249].

100 ppm in soil drench test gave 100% kill of the following: Fusarium solani, Phytophythora citrophthora, Rhizoctonia solani, Sclerotinia sclerotiorum, Sclerotium rolfsii [249].

10 ppm in soil drench test gave 100% kill of the following: Armillaria mellea, Phytophthora cactorum, P. cinnamoni, Phythium aphanidermatum, P. ultimum [249].

TOXICITY Man. Probable LD, 50-500 mg/kg [101]. May be irritating to eyes, skin and mucous membranes [101, 249].

50. CARBAMIC ACID, METHYLDITHIO-, SODIUM SALT (Concluded)

Animals. 285 mg/kg, p.o., produced acute toxicity in male albino mice, 820 mg/kg, p.o., in albino rats [249].

USE Agricultural: soil fungicide.

CAUTION Avoid skin contact, inhaling dust, mist, or fumes [249].

51. CARBANILIC ACID, ETHYL ESTER

ALTERNATIVE NAMES Ethyl carbanilate; Phenyl urethane.

MOLECULAR FORMULA $C_9H_{11}NO_2$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES Needles. Molecular weight, 165.186. Melting point, 52°C. Slightly decomposes at 238°C. Specific gravity, 1.106 (30/4°C). [118] Refractive index, 1.5105. Soluble in alcohol, ether, propylene glycol, peanut oil, olive oil, benzene. Slightly soluble in hexane. Insoluble in petroleum ether, chloroform, carbon tetrachloride, cold water.

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 5% solution of test compound prevented decay in fruit; slight rind injury [295].

TOXICITY Mice: LD_{50}, approximately 350 mg/kg, i.p.; LD, 400 mg/kg, i.v. [47].

USE Agricultural.

52. CARBANILIC ACID, THIONO-, ETHYL ESTER

ALTERNATIVE NAME Ethyl N-phenyl thiocarbamate.

MOLECULAR FORMULA $C_9H_{11}NOS$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES White solid. Molecular weight, 181.252. Soluble in peanut oil. Moderately soluble in propylene glycol.

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in solution of test compound, dried, and stored 3 weeks at 70°F. 5% solution prevented decay; no rind injury. 1¼% solution: 5 decayed, no rind injury. [293]

TOXICITY Mice: MTD, 500 mg/kg/da, i.p. for 5 days [136]; LD_{50}, 800 mg/kg, i.p. [266].

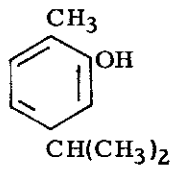
USE Protectant of materiel; agricultural.

53. CARVACROL

ALTERNATIVE NAMES Oxycymol; Isothymol; Isopropyl-o-cresol; 2-Hydroxy-p-cymene.

MOLECULAR FORMULA $C_{10}H_{14}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [53, 118], oily liquid [118, 220]. Thymol odor [53, 192]. Molecular weight, 150.212. Boiling point, 237.7°C [228], 237-238°C [220]. Specific gravity, 0.976 [192]. Refractive index, 1.52295 [118, 192, 220]. Soluble in alcohol, ether, alkalies. Insoluble in water. [53]

TESTS In vitro. Aspergillus niger: 250 ppm inhibited growth 100%; 100 ppm, 54%; 50 ppm, 29%. Trichoderma T-1: 250 ppm inhibited growth 100%. [228]

53. CARVACROL (Concluded)

TOXICITY Man. Probable LD, 50-500 mg/kg [101].

Animals. Salmo trutta (brown trout): 2 fish; test compound concentration, 5 ppm by weight. Death in 4 hours. Same test produced sickness in 4 hours in Lepomis macrochirus (bluegill sunfish), and Carassius auratus (goldfish). [297]

Animal	LD, mg/kg	Route
Cat	100	p.o.
Rabbit	100	p.o.
Rabbit	1000	s.c.
Frog	75	s.c.

[120]

COMPARATIVE TOXICOLOGY Somewhat less toxic than thymol in rats and rabbits [101].

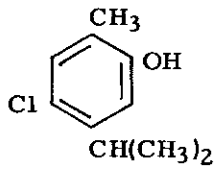
USE Protectant of materiel.

54. CARVACROL, 5-CHLORO-

ALTERNATIVE NAMES 4-Chloro-2-methyl-5-isopropyl phenol; 3-Isopropyl-4-chloro-6-methylphenol.

MOLECULAR FORMULA $C_{10}H_{13}ClO$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Crystalline powder. Molecular weight, 184.661. Melting point, 62-64°C [222]. Boiling point, 136-137°C (10 mm Hg). Specific gravity, 1.129. Refractive index, 1.5439. Soluble in organic solvents, alkalies; water, 1:1000.

TESTS In vitro. Trichophyton (gypseum) mentagrophytes, strain 640: Test compound added to culture undiluted. Significantly decreased infestation. Radius of inhibited zone, 4.5 cm after 1 week incubation. [248]

Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 1000 ppm of test compound inhibited spore germination (MED). [53]

Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 100% in 96 hours [229].

54. CARVACROL, 5-CHLORO- (Concluded)

Other organisms susceptible in vitro: Epidermophyton floccosum (Harz) Langeron and Milochevitch, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, T. (purpureum) rubrum (Castellani) Sabouraud, T. (Achorion) schoenleinii (Lebert) Langeron and Milochevitch, T. tonsurans, and T. (Achorion) violaceum Sabouraud. [222]

TOXICITY Man. Primary skin irritant [222].

USE Medicinal; agricultural. [125]

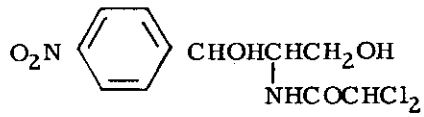
55. CHLORAMPHENICOL

ALTERNATIVE NAMES D-Threo-N-1,1-dihydroxy-1-p-nitrophenylisopropyl-dichloroacetamide; D(-)Threo-2-dichloroacetamido-1-p-nitrophenyl-1,3-propanediol; Chloromycetin; D(-)Threo-1-(p-nitrophenyl)-2-dichloroacetamido-1,3-propanediol; D(-)Threo-2,2-dichloro-N-[β-hydroxy-α-(hydroxymethyl)-p-nitrophenethyl acetamide].

SOURCE From soil bacterium Streptomyces venezuelae.

MOLECULAR FORMULA $C_{11}H_{12}Cl_2N_2O_5$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Fine, white to gray-white, or yellow-white, needle-like crystals or elongated plates. Bitter taste. [53] Molecular weight, 323.136. Melting point, 150.5-151.5°C. Sublimes in high vacuum. [192] Freely soluble in alcohol, propylene glycol, acetone, ethyl acetate, ether, methanol, ethanol, butanol. Very slightly soluble in water. Insoluble in benzene, petroleum ether, vegetable oils. [53,73,192] Reasonably stable in neutral or slightly acid solutions [53]. Thermostable, alkali labile [121]. Resists boiling water. Saturated aqueous solutions (0.25%) can be kept unaltered for months when refrigerated, but weaker solutions deteriorate. [105] Neutral to litmus [53].

TESTS In vitro. Compound inactive against most pathogenic yeasts and fungi, but inhibits growth of Actinomyces bovis [105]. Cryptococcus neoformans, and Nocardia asteroides also inhibited [222].

TOXICITY Man. Thrombocytopenia, granulocytopenia, and aplastic anemia are chief hematopoietic disturbances, the absolute incidence being low [105,222]. Oral doses of 1-2 g/da for 10 days or more, were well tolerated. Side reactions, (e.g., nausea, headache, skin eruptions and enteritic symptoms) have been relatively rare and minor. An occasional side effect, also occurring with other orally administered antibiotics, is stomatitis. Initial oral doses of 2.0 g, followed 8 hours later by 0.5 g, produced blood

levels of 9-13 μg/ml in 2 hours, leveling off to 5 μg/ml at 8 hours, with subtherapeutic concentrations thereafter. [121]

Animals. Mice tolerated for 2 weeks 385 mg/kg/da in diet, 100 mg/kg, s.c., and 250 mg/kg, i.p. Dogs tolerated daily oral doses of >200 mg/kg for over 4 months, or daily i.v. doses of 25-50 mg/kg. No cumulative toxic effect observed in hemopoiesis, liver and kidney function, or visceral tissues. Compound readily absorbed following parenteral and oral administration, and was found in blood, urine, bile, and cerebrospinal fluid 2 hours after intravenous, and 12-16 hours after oral, administration. S.c. doses of 100 mg/kg given twice daily produced blood concentrations of 11 μg/ml, and 60 μg/ml urine levels, in mice. [121]

Animal	LD_{50}, mg/kg	Route	Vehicle
Dog	>300	p.o.	Powder, by capsule
Dog	150	i.v.	Fermentation, 75-80% propylene glycol
Dog	101	i.m.	Fermentation, peanut oil
Dog	>46.5	i.m.	Fermentation, 62% propylene glycol
Mouse	2640	p.o.	Fermentation, acacia water suspension
Mouse	1320	i.p.	Fermentation, acacia water suspension
Mouse	109.5	i.v.	Fermentation, 25-28% propylene glycol
Mouse	195.4	i.v.	Fermentation, water
Mouse	202.6	i.v.	Synthetic
Rabbit	117	i.v.	Fermentation, 100% propylene glycol
Rat	175.5	i.v.	Fermentation, 60% propylene glycol
Rat	170.5	i.v.	Synthetic, 60% propylene glycol
Rat	279.4	i.v.	Fermentation, 50% acetamide
Rat	278.0	i.v.	Synthetic, 50% acetamide

[47]

USE Medicinal.

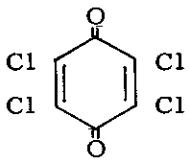
CAUTION As with other antibiotics, use of chloramphenicol may result in an overgrowth of microorganisms not susceptible to the drug, especially Monilia spp [105].

56. CHLORANIL

ALTERNATIVE NAMES Tetrachloroquinone; Tetrachloro-p-benzoquinone.

MOLECULAR FORMULA $C_6Cl_4O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow leaflets or prisms [318]. Molecular weight, 245.888. Melting point, 294-295°C [318], 285-287°C [118]. Soluble (g/100 g solvent at 25°C) in water, <0.008; acetone, 33; acetic acid, <0.009; benzene, <0.02; chloroform, <0.02; diethyl ether, 16; ethanol, 21; n-heptane, <0.02; mineral oil, <0.03; toluene, <0.02 [318]. Soluble in hot alcohol, ether [118, 228]. Slightly soluble in carbon disulfide, carbon tetrachloride. Insoluble in cold alcohol [228]. Stable to acids [180].

TESTS In vitro. Alternaria oleracea Milb., and Sclerotinia fructicola (Wint.) Rehm.: American Phytopathological Society glass slide test. 0.01-0.1 ppm of test compound inhibited spore germination. [189]

Aspergillus niger (Van Tiegham), and Chaetomium globosum: Test compound in 1% solution; also in saturated concentration, as well as the undiluted drug placed as a streak (bacto malt extract agar-1% yeast extract); incubated 72 hours at 30°C. All concentrations prevented infestation. [70]

Aspergillus niger (Van Tiegham), and Chaetomium globosum: 2% of test compound (dry cloth weight basis) on impregnated cloth prevented growth in 1-3 weeks. [70]

Aspergillus niger:

$\times 10^{-4}$ M	10	7.5	5.0	2.5	1.0
% inhibition	83	70	69	61	48

250 ppm inhibited growth 82%. [228]

	Concentration, M	% Inhibition
Penicillium citrinum	0.001	100
	0.0001	11
	0.00001	4
Trichoderma spp	0.001	70
	0.0001	3
	0.00001	0

[228]

TOXICITY Man. Not highly toxic [96]. Probable LD, 500-5000 mg/kg [101]. Gastrointestinal and skin irritation; liver and kidney damage [71]. Poor absorption [101].

Animals. Mice: 15.7 mg/kg, dissolved in peanut oil and administered i.p., daily for 5 days, resulted in death. 7.85 mg/kg, i.p., daily for 4 days, produced chronic toxicity but not death. 3.92 mg/kg, i.p., daily for 4 days, tolerated. [260] Rabbits: Test compound as dry dust, applied in excess to cornea of eye, caused corneal necrosis. 1:1 suspension provoked irritation when applied to clipped belly. [11] Rats: LD_{50}, approximately 4000 mg/kg, p.o.; 500 mg/kg, i.p. [120].

COMPARATIVE TOXICOLOGY Compound possesses enhanced fungicidal properties without the undesirable features of quinone, but is not as effective as 2,3-dichloro-1,4-napthoquinone (dichlone) [318].

USE Agricultural: seed protectant; downy mildew control. Protectant of materiel: leather preservative [111, 227].

57. CHLOROPICRIN

ALTERNATIVE NAMES Nitrotrichloromethane; Trichloronitromethane; Nitrochloroform.

MOLECULAR FORMULA CCl_3NO_2

STRUCTURAL FORMULA CCl_3NO_2

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [180]; slightly oily liquid [53]. Molecular weight, 164.389. Melting point, -69.2°C [53], -64°C [118, 180]. Boiling point, 112°C [53]. Vapor pressure, 5.7 mm Hg (0°C), 23.8 mm Hg (25°C) [180]. Specific gravity, 1.651 [118], 1.692 (0°C) [53]. Refractive index, 1.4595 [180], 1.46075 (23°C) [118]. Soluble in alcohol, benzene, carbon disulfide. Slightly soluble in ether. Relatively stable [53].

TOXICITY Man. Extremely toxic. Probable LD, 5-50 mg/kg. [97] A powerful irritant; affects all body surfaces; causes lachrimation, vomiting, bronchitis, pulmonary edema. Inhalation causes anemia, weak and irregular heart beat, recurrent asthmatic attacks. [71, 101, 250]

Animals. Very toxic when inhaled or swallowed.

Animal	Dose	mg/kg	Route	Time of Death
Cat	LD	10[1]	s.c.	6 da
Rabbit	MLD	10[2]	i.v.	
Rabbit	LD	500	i.p.	20 min-2 hr

[120]

Animal	LC, mg/L	ppm	Exposure Time	Time of Death
Cat	0.8	110	20 min	14 da
Guinea pig	0.8	110	20 min	2 da
Rabbit	0.8	110	20 min	3 da
Rabbit	5	743	Continuous	30 min

[120]

USE Agricultural: Effective against most soil-borne pathogenic fungi except the sclerotia-forming types [180].

CAUTION Handlers should wear protective clothing, chemical safety goggles, respirator [250].

/1/ In alcohol. /2/ Emulsion in water.

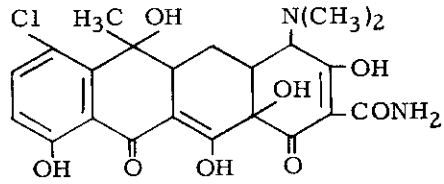
58. CHLORTETRACYCLINE

ALTERNATIVE NAMES Aureomycin; Duomycin.

SOURCE Streptomyces aureofaciens (Duggar).

MOLECULAR FORMULA $C_{22}H_{23}ClN_2O_8$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Golden yellow crystals [53, 192]. Odorless [302]. Bitter taste. Molecular weight, 478.877. Melting point (free base), 168-169°C (uncorr.). Decomposes above 210°C. [53] Soluble in "Cellosolve," dioxane, "Carbitol." Slightly soluble in alcohol, acetone, benzene. [222] Stable in air, but strong sunlight causes darkening [53].

TOXICITY Man. Rare cases of hypersensitivity. Occasional diarrhea, skin eruptions. [222] Anorexia, nausea, vomiting, skin eruptions, vaginitis, pruritus [192].

Animals.

Animal	LD_{50}, mg/kg	Route
Dog	150	i.v. (rapid)
Mouse	2500	p.o.
Mouse	>3000	p.o.
Mouse	3000-4000	s.c.
Mouse	50-100	i.v.
Mouse	155(140-172)	i.v.
Mouse	134[1]	i.v.
Mouse	102[2]	i.v.
Mouse	130	i.v.
Mouse	192(145-250)	i.p.
Rat	>3000	p.o.
Rat	160(150-170)	i.v.
Rat	118[1]	i.v.
Rat	335(305-369)	i.p.

[47]

USE Medicinal: systemic mycoses [252]. Protectant of materiel.

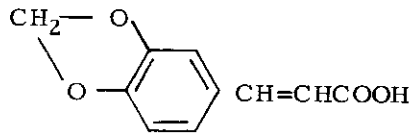
/1/ pH 2.5. /2/ pH 8.5

59. CINNAMIC ACID, 3,4-METHYLENEDIOXY-

ALTERNATIVE NAME 3,4-Methylenedioxycinnamic acid.

MOLECULAR FORMULA $C_{10}H_8O_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 192.164. Melting point, 240°C. Insoluble in alcohol, acetone, water.

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm completely inhibited spore germination. Stemphylium sarcinaeforme Cav.: 100 μg/sq cm completely inhibited spore germination. [53]

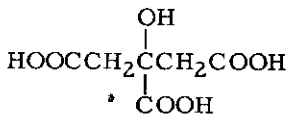
USE Agricultural.

60. CITRIC ACID

ALTERNATIVE NAMES β-Hydroxytricarballylic acid; 2-Hydroxy-1,2,3-propanetricarboxylic acid.

MOLECULAR FORMULA $C_6H_8O_7$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless, translucent crystals, or as a white granular to fine crystalline powder. Odorless. Strongly acid taste. [53] Molecular weight, 192.124. Melting point, 153°C. Specific gravity, 1.542 (18/4°C). Soluble in alcohol, water, acetone. [118] Hydrated form is efflorescent in dry air [53].

TOXICITY Man. Reported to cause allergic symptoms [250].

Animals. Dogs given 1380 mg/kg in capsule form, daily for 112-120 days, showed no symptoms or evidence of renal damage. 5% in diet of rats for 2 years had no effect on survival. [171]

60. CITRIC ACID (Concluded)

Animal	LD_{50}, mg/kg	Route	Reference
Mouse	46.2[1]	i.v.	120
Mouse	203[2]	i.v.	171
Mouse	1050	i.p.	120
Rabbit	360[2]	i.v.	120
Rat	975	i.p.	120

USE Agricultural.

61. COPPER CARBONATE, BASIC

ALTERNATIVE NAMES Cupric carbonate; Artificial malachite.

MOLECULAR FORMULA $CH_2Cu_2O_5$

STRUCTURAL FORMULA $CuCO_3 \cdot Cu(OH)_2$

PHYSICAL AND CHEMICAL PROPERTIES Green [53,179], dark green [118] powder [53,179]. Molecular weight, 221.106. Decomposes, 200°C. Specific gravity, 3.7-4.0 [53], 4 [118]. Refractive index, 1.655 [118]. Soluble in acids [53]. Insoluble in water, alcohol [118].

TOXICITY Man. Irritating and corrosive [191].

COMPARATIVE TOXICOLOGY Slightly less effective than copper sulfate as seed fungicide [95].

USE Agricultural: smut preventive [53]; control of wheat bunt [95]; fungicide for cereal seeds [179].

62. CREOSOTE

ALTERNATIVE NAMES Wood tar creosote; Wood creosote.

PHYSICAL AND CHEMICAL PROPERTIES Almost colorless or yellowish, oily liquid. Smoky odor. Burning taste. [192] Boiling point, approximately 203°C [192], 205-220°C [53]. Specific gravity, 1.080 [53]; not below 1.076 (25/25°C) [192]. Soluble in glycerol, glacial acetic acid, fixed alkaline hydroxide solutions. Miscible with alcohol, chloroform, ether, oils. [192]

/1/ Rapid injection. /2/ Slow injection.

62. CREOSOTE (Concluded)

TOXICITY Man. Probable LD, 50-500 mg/kg [101]; established fatal dose, 10 g [71]. May cause cardiovascular collapse [192]; CNS stimulation, convulsions; CNS depression, coma; GI and skin irritation; blood pressure fall. [71] Treated woods and ropes reported to have irritated hands of users [250].

COMPARATIVE TOXICOLOGY Toxic action similar to that of phenol [101].

USE Protectant of materiel: wood [99, 111], textiles [111].

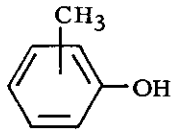
CAUTION Use only with adequate ventilation. Individuals handling compound should wear protective equipment: chemical safety goggles, respirator, protective clothing. [250]

63. CRESOL

ALTERNATIVE NAMES Methylphenol; Cresylic acid.

MOLECULAR FORMULA C_7H_8O

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless, yellowish-pink, or brown, oily liquid. Phenol-like odor. [53] Molecular weight, 108.134. Distills between 195-205°C. Specific gravity, 1.030-1.038 [53, 302]. Highly refractive. Soluble in alcohol, ether, glycol, dilute alkalies. Miscible with water and alcohol. Darkens with age and exposure to light. Saturated solution neutral or slightly acid to litmus. [53]

TOXICITY Man. Rapidly absorbed through skin. Causes severe burns. Collapse and exhaustion followed by coma and death; sometimes marked alterations in liver, with nephritis and hemolysis. [59]

COMPARATIVE TOXICOLOGY Toxic action similar to that of phenol [250].

USE Medicinal; protectant of materiel; agricultural. [125, 192]

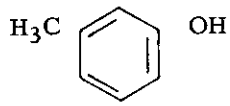
CAUTION Individuals exposed to compound should use protective equipment [250].

64. m-CRESOL

ALTERNATIVE NAMES 3-Methylphenol; m-Cresylic acid; m-Hydroxytoluene.

MOLECULAR FORMULA C_7H_8O

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [228] to yellow [192] liquid [228]. Phenol-like odor [192]. Molecular weight, 108.134. Melting point, 8-10.9°C [228]. 11.5°C [72], 11-12°C [118]. Boiling point, 202°C [228], 202.2°C [72], 202.8°C [118]. Specific gravity, 1.034 [118]. Vapor pressure, 0.1930 mm Hg (25°C) [72]. Refractive index, 1.5364 [228], 1.5398 [118], 1.5438 [72]. Miscible with alcohol, ether, benzene, carbon tetrachloride, acetone [72]. Slightly soluble in water [53].

TESTS In vitro. Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	23				
	25	18	16	11	6
	39	32	23	11	9

[228]

TOXICITY Man. Probable LD, 50-500 mg/kg [97]. Readily absorbed through skin; causes severe burns. [192]

Animals.

Animal	Dose	mg/kg	Route	Time of Death
Cat	LD	180[1]	s.c.	27 hr
Dog	LD	150	i.v.	
Guinea pig	LD	300-400	s.c.	
Guinea pig	LD	100	i.p.	6-8 hr
Mouse	LD_{50}	168	i.p.	
Mouse	LD	450	s.c.	
Rabbit	LD	1400[2]	p.o.	8 hr
Rabbit	LD	500-600	s.c.	2-12 hr
Rabbit	LD	280[3]	i.v.	15 hr
Rat	LD_{50}	2020	p.o.	
Rat	LD	900	s.c.	
Frog	LD	250	s.c.	12-24 hr

[120]

/1/ 10% solution in olive oil. /2/ 20% solution in water. /3/ 0.5% solution in water.

64. m-CRESOL (Concluded)

COMPARATIVE TOXICOLOGY m-Cresol has approximately same toxic action as phenol; perhaps slightly more corrosive than phenol, but systemic effects may be somewhat milder because of slower absorption. [101]

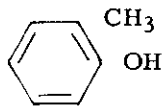
USE Protectant of materiel: size and fiber preservative; mildew preventive. [125]

65. o-CRESOL

ALTERNATIVE NAMES o-Methylphenol; o-Hydroxytoluene; o-Cresylic acid.

MOLECULAR FORMULA C_7H_8O

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless, yellowish, brownish-yellow or pink [192], crystals or liquid [228]. Phenolic odor [192]. Molecular weight, 108.134. Melting point, 30°C [118], 29-31°C [228]. Boiling point, 190.95°C [72], 191°C [228]. Specific gravity, 1.0465. Refractive index, 1.5453 (25°C). [118] Vapor pressure, 0.4254 mm Hg (25°C). Soluble in alcohol, ether, acetone, carbon tetrachloride, benzene, n-heptane. Slightly soluble in water. [72] Darkens with age or with exposure to light [192].

TESTS In vitro. Aspergillus niger: 250 ppm inhibited growth 52-58% [228].

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard: 2,500,000 conidia per plate; Sabouraud's dextrose agar plus 10% horse serum; 1 cc of 0.1% alcohol solution of test compound in agar; incubated 5 days at 28-30°C. Decreased infestation. Agar disks from 15-day culture, in 1% solution of test compound for 1 minute, rinsed, subcultured on Sabouraud's medium 21 days. Did not abolish growth. [312]

TOXICITY Man. Rapidly absorbed through skin; causes severe burns [53].

Animals.

Animal	Dose	mg/kg	Route	Time of Death
Cat	LD	55[1]	s.c.	60 hr
Dog	LD	80	i.v.	
Guinea pig	LD	350-400	s.c.	
Guinea pig	LD	350	i.p.	70 min
Mouse	LD	350	s.c.	
Rabbit	LD	940[2]	p.o.	4 hr
Rabbit	LD	450-500	s.c.	<2-3 hr

(continued)

/1/ 10% solution in olive oil. /2/ 20% emulsion in water.

65. o-CRESOL (Concluded)

Animal	Dose	mg/kg	Route	Time of Death
Rabbit	LD	180[1]	i.v.	8 hr
Rat	LD_{50}	1350	p.o.	
Rat	LD	650	s.c.	
Frog	LD	200	s.c.	

[120]

COMPARATIVE TOXICOLOGY o-Cresol more toxic than m-cresol [101].

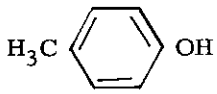
USE Protectant of materiel: size and fiber preservative; mildew preventive. [125] Medicinal: treatment of superficial mycoses (aqueous solution, 2-5%) [252].

66. p-CRESOL

ALTERNATIVE NAMES 4-Methylphenol; p-Cresylic acid; p-Hydroxytoluene.

MOLECULAR FORMULA C_7H_8O

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless prisms [118]. Phenolic odor [192]. Molecular weight, 108.134. Melting point, 28-32°C [228], 34.78°C [72]. Boiling point, 201.92°C [72], 202-202.1°C [228], 202.5°C [118]. Specific gravity, 1.0347 [118], 1.0788 (41°C), 1.0295 (25°C) [228]. Refractive index, 1.5395 [118, 192], 1.53115 (41°C) [72]. Soluble in alcohol, ether, chloroform. Slightly soluble in water. [53]

TESTS In vitro. Aspergillus niger (Van Tiegham): Test compound in nutrient medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7); incubated 48 hours at 37°C. 0.06% concentration inhibited growth (MED). [181]

A. niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	36	29	23	15	7

[228]

/1/ 0.5% solution in water.

66. p-CRESOL (Concluded)

TOXICITY Man. Rapidly absorbed through skin; causes severe burns. [46]

Animals.

Animal	Dose	mg/kg	Route	Time of Death
Cat	LD	80[1]	s.c.	120 hr
Guinea pig	LD	200-300	s.c.	
Guinea pig	LD	100	i.p.	6-22 hr
Mouse	LD_{50}	24.8	i.p.	
Mouse	LD	150	s.c.	
Rabbit	LD	620[2]	p.o.	4 hr
Rabbit	LD	300-400	s.c.	12-36 hr
Rabbit	LD	180[3]	i.v.	15 hr
Rat	LD_{50}	1800	p.o.	
Rat	LD	500	s.c.	
Frog	LD	150	s.c.	

[120]

COMPARATIVE TOXICOLOGY p-Cresol more toxic than m-cresol [101].

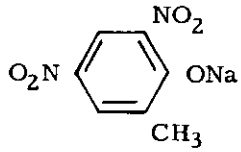
USE Protectant of materiel: size and fiber preservative; mildew preventive. [125]

67. o-CRESOL, 4,6-DINITRO-, SODIUM DERIVATIVE

ALTERNATIVE NAMES Sodium 4,6-dinitro-o-cresoxide; 4,6-Dinitro-o-cresol; DNOC; 4,6-Dinitro-2-methyl phenol.

MOLECULAR FORMULA $C_7H_5N_2O_5 \cdot Na$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow solid [53]. Molecular weight, 220.123. Melting point, 85.8°C. Very slightly soluble in water. [53]

TOXICITY Man. Toxic when inhaled, may be fatal if swallowed. Burning in throat, shock, respiratory failure; irritating to eyes and skin. [190] Principal manifestation is elevation of body temperature [71].

/1/ 10% solution in olive oil. /2/ 20% emulsion in water. /3/ 0.5% solution in water.

67. o-CRESOL, 4,6-DINITRO-, SODIUM DERIVATIVE (Concluded)

PHYTOTOXICITY Highly toxic and cannot be used successfully on actively growing plants [53].

USE Agricultural: asparagus rust; fruit tree spray. [144]

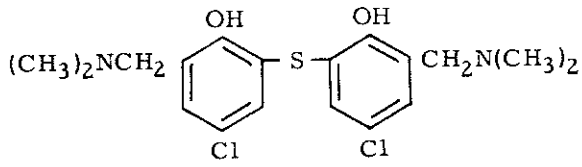
CAUTION Use respirator when handling [96].

68. o-CRESOL, 6,6'-THIOBIS(4-CHLORO-α-DIMETHYLAMINO)-

ALTERNATIVE NAME 3-β-17-[Bis-(2-hydroxy-3-dimethyl-aminomethyl-5-chloro-phenyl)sulfide].

MOLECULAR FORMULA $C_{18}H_{22}Cl_2N_2O_2S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 401.352. Melting point, 55-57.5°C. Soluble in methyl alcohol, acetone. Insoluble in water.

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: 10-fold dilutions of test compound added to spore suspension in depression slide cavity; incubated 17 hours.

μg/sq cm	% Inhibition
1000	100
100	100
10	100
1	100

[55]

TOXICITY MTD in mice, 200 mg/kg, p.o. [38].

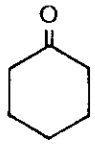
USE Agricultural.

69. CYCLOHEXANONE

ALTERNATIVE NAMES Ketohexamethylene; Pimelic ketone.

MOLECULAR FORMULA $C_6H_{10}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]. Acetone- and peppermint-like odor [192]. Molecular weight, 98.140. Freezing point, -45 to -30°C [228]. Boiling point, 156.7°C [118]. Vapor pressure, 136 mm Hg (100°C) [53]. Specific gravity, 0.9478 [53,118]. Refractive index, 1.4503 [228], 1.4507 [53,118]. Miscible with most solvents [53].

TESTS In vitro.

	ppm	% Inhibition
Aspergillus niger (Van Tiegham)	1000	0
	250	-16
	100	32
Trichoderma T-1	1000	20
	100	0
Penicillium citrinum	1000	44
	100	6

[228]

TOXICITY Man. Weak CNS depressant, mild or moderate irritant [71,101]. 50 ppm not tolerated (throat irritation most marked effect); 25 ppm tolerated. [250]

Animals.

Animal	Dose	mg/kg	Route
Mouse	MLD	1300-1500	i.p.
Rabbit	MLD	1600-1900	p.o.
Rabbit	MLD	10,200-23,000	c.t.
Rat	LD_{50}	3460(2810-4260)	p.o.

[120]

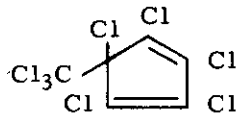
USE Protectant of materiel: leather [107].

70. CYCLOPENTADIENE, 1,2,3,4,5-PENTACHLORO-5-(TRICHLOROMETHYL)-

ALTERNATIVE NAME Octachloromethylcyclopentadiene.

MOLECULAR FORMULA C_6Cl_8

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White solid. Molecular weight, 355.716. Melting point, 183°C. Soluble in benzene, carbon tetrachloride. Slightly soluble in ethanol. Insoluble in water. Converted to hexachlorobenzene at 350-400°C.

TESTS In vitro.

	µg/sq cm	% Inhibition
Stemphylium sarcinaeforme Cav.	1000	100
	100	100
	10	100
	1	0
Sclerotinia fructicola (Wint.) Rehm.	1000	100
	100	100
	10	0

[55]

TOXICITY Salmo trutta (brown trout), and Lepomis macrochirus (bluegill): 5 ppm, by weight, of test compound. Death after 23 hours. [297]

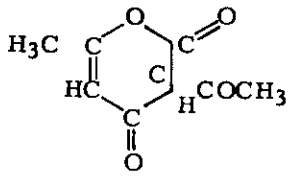
USE Agricultural.

71. DEHYDROACETIC ACID

ALTERNATIVE NAMES DHA; 3-Acetyl-6-methyl-2(H)-pyran-2,4(3H)dione; 2-Acetyl-5-hydroxy-3-oxo-4-hexenoic acid delta-lactone; 3(1-Hydroxyethylidene-6-methyl-2(H)-pyran-2,4(3H)-dione.

MOLECULAR FORMULA $C_8H_8O_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless crystals [53]; rhombic needles or plates [118]. Odorless [53, 180]. Tasteless [53]. Molecular weight, 168.144. Melting point, 108.5°C [53], 109°C [118]. Sublimes, 109-111°C. Boiling point, 269.9°C [180], 270°C [118]. Soluble in hot alcohol [118]; acetone, ether, alkalies [180]. Insoluble in water [180].

TESTS In vivo. Monilinia fructicola (Wint.) Honey (brown rot): Reduced 50% in peaches by 1% spray; 83% by 2% spray. [116]

TOXICITY Man. 0.01 g/kg for 150 days produced no ill effects [101]. Non-irritating to skin, no evidence of sensitization [180].

Animals. Loss of weight in rats fed 0.3 g/kg for 34 days; no ill effects at 0.1 g/kg for over 2 years. [180] High dosage levels produced anorexia, vomiting, weakness, stupor, ataxia, and convulsions in monkeys [101].

Animal	Dose	mg/kg	Route	Reference
Dog	LD	400[1,2]	p.o.	120
Dog	LD	400[1,2]	i.v.	120
Mouse	LD_{50}	2000	i.p.	120
Rat	LD_{50}	1000	p.o.	47, 180
Rat	LD_{50}	1000[3]	p.o.	120
Rat	LD_{50}	570[1,2]	p.o.	120

COMPARATIVE TOXICOLOGY As toxic as phenol [180].

USE Agricultural: prevention of mold growth in fruits [180], cosmetics and food stuffs [125]. Medicinal [53].

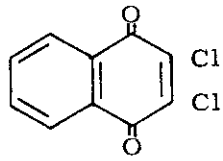
/1/ As sodium salt; calculated as acid equivalent. /2/ In water. /3/ Olive oil emulsion in gum arabic.

72. DICHLONE

ALTERNATIVE NAME 2,3-Dichloro-1,4-naphthoquinone.

MOLECULAR FORMULA $C_{10}H_4Cl_2O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals [95]. Molecular weight, 227.046. Melting point, 194°C. Soluble (g/100 g solvent at 25°C) in acetone, 2.2; acetic acid, 0.85; benzene, 3.2; chloroform, 2.9; diethyl ether, 0.6; ethanol, 0.15; n-heptane, 0.06; mineral oil, 0.12; toluene, 3.5; water, <0.008. [185] Moderately soluble in xylene, o-dichlorobenzene [180].

TESTS In vitro. Alternaria oleracea Milb. and Sclerotinia fructicola (Wint.) Rehm.: Spores placed on treated glass slide for germination test. 0.001-0.1 ppm inhibited germination about 50%. [189]

Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 10 ppm inhibited spore germination. [55]

Aspergillus niger (Van Tiegham): LD_{50}, 3 ppm; LD_{84}, 70 ppm [229].

A. niger:

ppm	% Inhibition
0.5	21
1.0	23
2.5	40
5.0	73
10.0	100

[229]

In vivo. Alternaria solani (Ell. and Mart.) J. and G.: Infected tomato plants sprayed with 80-100 ppm. Controlled foliage infection (ED_{95}). [189]

Pythium spp (on seeds and vegetables), Phytophthora infestans (potato blight), Venturia inaequalis (Cooke) Winter (apple scab), Sclerotinia fructicola (Wint.) Rehm. (brown rot of stone fruits), Colletotrichum lindemuthianum (bean anthracnose), Gymnosporium juniper-virginianae (cedar apple rust): Compound is effective protectant. [189]

Phomopsis citri, and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges, dipped in compound, and stored. Saturated solution did not control disease; did not produce significant injury to rind on controls. [295]

72. DICHLONE (Concluded)

TOXICITY Man. Probable LD, 500-5000 mg/kg [101]. Skin irritant under warm conditions [180]. GI and skin irritation, liver and kidney damage [71].

Animals. Rats: LD_{50}, 1300 mg/kg, p.o. 1580 ppm in diet for 2 years had no effect. [180] Diarrhea and severe CNS depression [101].

Skin irritation enhanced by fats and oils. Large doses promptly vomited by dogs. [101]

PHYTOTOXICITY Non-toxic to plants [95, 180].

COMPARATIVE TOXICOLOGY Reported to be 4-8 times as effective as chloranil against certain fungi [95].

USE Protectant of materiel [125]. Agricultural: seed protectant; foliage spray [95, 180].

73. DIETHYLAMINE, 2,2'-DICHLORO-N-METHYL-, HYDROCHLORIDE

ALTERNATIVE NAMES Mechlorethamine hydrochloride; HN_2 hydrochloride; MBA hydrochloride; Nitrogen mustard; Dichloren; T-1024; Mustine; Mustargen hydrochloride.

MOLECULAR FORMULA $C_5H_{11}Cl_2N \cdot HCl$

STRUCTURAL FORMULA $(ClCH_2CH_2)_2NCH_3 \cdot HCl$

PHYSICAL AND CHEMICAL PROPERTIES White crystals. Molecular weight, 192.525. Very soluble in water. Soluble in alcohol [192]. Relatively stable in 10% aqueous solution at low temperatures.

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 250 ppm inhibited growth 100%. [281]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, strain 640: Melted agar, seeded with conidia, allowed to harden. A small portion of the chemical was placed on the plate in a 3-5 mm area; if liquid, chemical was put in a glass cylinder. Plates incubated at 30°C and zone of inhibition read at 1- and 2-week intervals. Untreated controls incubated under the same conditions. Width of zone of inhibition measured not only fungicidal action, but also diffusability of the material through the agar. Radius of inhibition zone, 0.3 cm. [281]

73. DIETHYLAMINE, 2,2'-DICHLORO-N-METHYL-, HYDROCHLORIDE (Concluded)

TOXICITY Man. Highly toxic, both locally and systemically [8]. Very irritating to mucous membranes. May produce nausea, vomiting, bloody diarrhea, leukopenia, anemia. Overdose may produce thrombocytopenia, severe leukopenia, hemorrhagic diathesis. [192]

Animals. Stimulation of central nervous system, intermittent convulsions, progressive muscular paralysis, anorexia, weight loss, profuse vomiting, hemorrhagic enteritis with diarrhea, depression of hematopoiesis, disturbances of electrolyte and water balance [8].

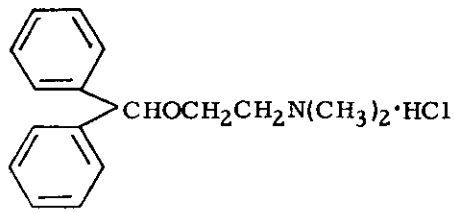
USE Medicinal.

74. DIPHENHYDRAMINE HYDROCHLORIDE

ALTERNATIVE NAMES Amidryl; 2-(Benzhydryloxy)-N, N-dimethylethylamine hydrochloride; β-Dimethylaminoethyl benzhydryl ether hydrochloride.

MOLECULAR FORMULA $C_{17}H_{21}NO \cdot HCl$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals. Odorless [53, 83, 302]. Bitter taste [83]. Molecular weight, 291.811. Melting point, 166-170°C [53]. Freely soluble in water, alcohol, chloroform. Slightly soluble in acetone, benzene, ether. [53] Stable under ordinary conditions of temperature and atmosphere. Darkens slowly on exposure to light. [53, 201] Neutral to litmus [83].

TESTS In vitro. Coccidioides immitis, 3 strains: Inocula were saline suspensions of spores collected from cultures on 2% glucose and 1% yeast extract agar (5×10^4 cells per ml). "Benadryl" and "Pyribenzamine," containing test compound were made up in saline solutions, adjusted to pH 7.3, and sterilized by Seitz filtration. In those instances recorded as no "growth," viability tests proved that cultures had not been sterilized and that the action was primarily fungistatic.

Concentration, M	Strain of Coccidioides immitis[1]		
	Silveira	Cash	PW
Benadryl			
0.0002	+	+	+
0.0004	-	-	-
0.0008	-	-	-
0.0016	-	-	-
Pyribenzamine			
0.0002	+	+	+
0.0004	+	+	+
0.0008	+	+	+
0.0016	-	-	-

[224]

TOXICITY Man. Probable LD, 5-50 mg/kg[101]. Drowsiness, dizziness, weakness, nausea, vertigo, dry mouth, confusion, muscular twitching, dilatation of pupils, narcolepsy, palpitation, malaise, disturbed vision, followed by convulsions, collapse, death. [119,154,192]

Animals.

Animal	LD_{50}, mg/kg	Route	Reference
Dog	24	i.v.	120
Dog	91.3[2]	i.v.	47
Dog	79.9[3]	i.v.	47
Guinea pig	284.0	p.o.	47
Guinea pig	40.2	s.c.	47
Guinea pig	75	i.p.	120
Hamster	18	i.v.	120
Mouse	164	p.o.	120
Mouse	114.1	p.o.	47
Mouse	127	s.c.	120
Mouse	148 ± 8	s.c.	120
Mouse	116.1	s.c.	47
Mouse	75 ± 5.2	i.p.	120
Mouse	80 ± 8	i.p.	120
Mouse	83-85	i.p.	120
Mouse	74.6	i.p.	120
Mouse	56.7	i.p.	47
Mouse	31 ± 0.8	i.v.	120
Mouse	35 ± 1	i.v.	120
Mouse	32	i.v.	47
Mouse	55.0	i.v.	47
Rabbit	10	i.v.	120

(continued)

/1/ (+) = visible growth; (-) = inhibition. /2/ Salt. /3/ Base.

74. DIPHENHYDRAMINE HYDROCHLORIDE (Concluded)

Animal	LD_{50}, mg/kg	Route	Reference
Rat	500	p.o.	120
Rat	545	p.o.	120
Rat	474	s.c.	120
Rat	82	i.p.	120
Rat	61 ± 9	i.p.	120
Rat	42	i.v.	120
Rat	46	i.v.	120

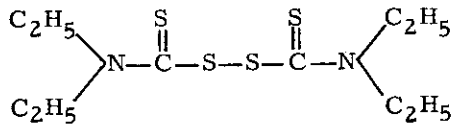
USE Medicinal [67].

75. DISULFIDE, BIS(DIETHYLTHIOCARBAMYL)-

ALTERNATIVE NAMES Antabuse; Ethyl thiurad; Thiuranide; Tetradine; Tetraetil; Esperal; Tetraethylthiuram disulfide; Disulfiram; Tetraethyl-X.

MOLECULAR FORMULA $C_{10}H_{20}N_2S_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Cream color [53], white to light gray [8], crystals [67]. Odorless [8]. Almost tasteless [8]; bitter taste [67]. Molecular weight, 296.540. Melting point, 65-70°C. Specific gravity, 1.17 (20/20°C). Soluble in carbon disulfide, benzene, chloroform [53]; alcohol [8]. Slightly soluble in acetone, lower alcohols. Insoluble in water. [8]

TESTS In vitro. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 10 μg/sq cm completely stopped spore germination. [55]

Sabouraud's agar (Difco) streaked with 10-day agar slant culture of test organism; test compound added and incubated 15 days at 25°C:

	MED, ppm
Trichophyton (gypseum) mentagrophytes	25
Candida albicans	25
Microsporum canis Bodin	50
Sporotrichum schenckii	50
Blastomyces dermatitidis	12.5

[195]

75. DISULFIDE, BIS(DIETHYLTHIOCARBAMYL)- (Concluded)

TOXICITY Man. 6 g tolerated without untoward symptoms unless alcohol also ingested; 5.5 g followed by 30 cc of rum resulted in death. Alcohol following drug causes intense vasodilatation of face and neck, increased respiration and pulse rate, nausea, pallor, hypotension, vomiting; large doses of alcohol cause dizziness, headache, palpitation, dyspnea, unconsciousness. [43]

Animals. Rats: Most prominent signs of toxicity are lethargy, anorexia, loss of weight, diarrhea, constipation, ascending paralysis, muscle wasting. LD_{50}, 8600 mg/kg, p.o., in aqueous suspension. Dogs: marked nausea and vomiting. 3500 mg/kg, p.o., lethal to 1 dog which vomited only a slight amount. Rabbits: LD_{50}, 1800 mg/kg, p.o. [43] Mice: 500 mg/kg, dissolved in butyl succinate and administered i.p. daily, did not produce death. 15.6-500 mg/kg, i.p., in butyl succinate, produced hypersensitivity to compound. [260]

Animal	Dose	mg/kg	Route
Dog	LD	3500[1]	p.o.
Rabbit	LD_{50}	1800 ± 130	p.o.
Rabbit	LD_{50}	2050	p.o.
Rat	LD_{50}	8600 ± 370	p.o.

[120]

USE Protectant of materiel; medicinal.

76. DISULFIDE, BIS(DIMETHYLTHIOCARBAMYL)-

ALTERNATIVE NAMES TMTDS; TMTD; Thiram; Thiurad; Tetramethyl thiuram disulfide; Bis(dimethylthiocarbamyl) disulfide.

MOLECULAR FORMULA $C_6H_{12}N_2S_4$

STRUCTURAL FORMULA $(CH_3)_2NC(:S)SSC(:S)N(CH_3)_2$

PHYSICAL AND CHEMICAL PROPERTIES White [53], yellow [118] dust, crystalline powder or grains. Molecular weight, 240.436. Melting point, 139-146°C [38], 146-148°C [53]. Soluble (g/100 g solvent at 25°C) in water, <0.005; acetone, 3.1; acetic acid, 0.16; benzene, 5.0; chloroform, 15; diethyl ether, <0.02; ethanol, 0.06; n-heptane, <0.008; mineral oil, <0.03; toluene, 1.6. Very soluble in carbon disulfide. Insoluble in dilute alkalies, gasoline. [318]

/1/ Approximately.

TESTS In vitro. Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 100% [229].

Spore germination test, Oxford cup method. Approximately 6 x 10^3 spores, or 1 drop of heavy suspension, incubated 3 days at 24°C. A. niger: MED, 3.5 ppm at pH 4.7-6.5. Growth of mycelium from spores completely inhibited at concentrations of 0.35-2 ppm, and at 5 or greater ppm. Botrytis cinerea Fr.: 0.15 ppm completely inhibited growth at pH 4.2-6.6. Penicillium italicum (Wehmer): 0.35 ppm completely inhibited growth at pH 4.6-7.2. Rhizopus nigricans (Ehrenberg): 0.15 ppm completely inhibited growth at pH 4.1-5.0. [147]

TOXICITY Man. Skin patch test: Application of dry powder produced very slight erythema in 9% of subjects. Soap containing compound proved irritating to 8 out of 309 subjects; developed allergic sensitization in 1 out of 214 cases. [13] Dust may be irritating to skin and mucous membranes [95].

Animals. Mice: Test compound administered in suspension of gum acacia in saline solution: 250 mg/kg, i.p., daily for 5 days, caused death; 125 mg/kg, i.p., daily for 5 days, tolerated. [260]

Rats: LD_{50}, 780 mg/kg, p.o. [161]; 860 mg/kg, p.o. [310]; 865 mg/kg, p.o. [268]. Test compound dissolved in propylene glycol: LD_{50}, approximately 500 mg/kg, s.t. [62].

Rabbits: LD_{50}, 210 mg/kg, p.o. [28]. 4 out of 6 survived 3 injections, and 2 out of 6 survived 4 injections, of 70 mg/kg, i.p. 24-hour contact gave moderate skin irritation. [28] Dry dust, or a 1:1 suspension in water, applied to clipped belly provoked skin irritation [184]. Lung tissue showed moderate irritation from concentrations ranging from 0.00127 mg/L, inhaled 24 hours per day for 30 days, to 0.0019 mg/L, inhaled 7 hours per day for 5 weeks [28]. Compound applied in excess to eye as dry dust, or 1:1 suspension in water, caused corneal necrosis [184].

Guinea pig: 42% aqueous paste moderately irritating to skin [161].

COMPARATIVE TOXICOLOGY Approximately 10 times as toxic as bis(diethylthiocarbamyl) disulfide [62].

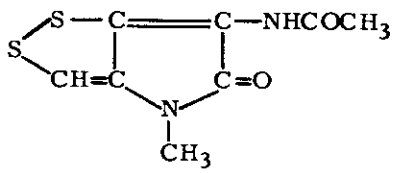
USE Protectant of materiel. Agricultural: turf diseases [125]; foliage, seeds [53, 180].

77. 1,2-DITHIOLO[4,3-b]PYRROL-5(4H)-ONE, 6-ACETAMIDO-4-METHYL-

ALTERNATIVE NAME Thiolutin.

MOLECULAR FORMULA $C_8H_8N_2O_2S_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Brilliant yellow needles [192]. Molecular weight, 228.292. Decomposes, 270°C [121]. Specific gravity, <1. Soluble in most organic solvents. Slightly soluble in water. Acid stable, alkali labile, thermostable. [121]

TESTS In vitro.

Inhibited Organism	Compound µg/ml
Histoplasma capsulatum	6.2
Microsporum audouini	12.5
Trichophyton rubrum	12.5
Epidermophyton floccosum	12.5
Coccidioides immitis	50.0
Paracoccidioides brasiliensis	50.0
Blastomyces dermatitidis	50.0

[121]

Candida albicans not sensitive. Species of Pythium, Sphaeropsis and Sclerotinia inhibited by 10 ppm; Colletotrichum, Phomopsis, Rhizoctonia by 50-100 ppm. [121]

In vivo. Concentrations up to 1% as dust markedly improved germination of oat grain infected with Helminthosporium sativum [121].

TOXICITY LD_{50} in mice, 25 mg/kg, s.c.; 25 mg/kg, p.o. [121]

PHYTOTOXICITY 100 ppm non-toxic to leaves of young tomato plants, roots of maize, pea, tomato, sunflower, and to seeds of maize, pea or radish [121].

USE Medicinal; agricultural.

78. ETHANE, 1,2-DIBROMO-

ALTERNATIVE NAMES 1,2-Dibromoethane; Ethylene dibromide; EDB; Ethylene bromide.

MOLECULAR FORMULA $C_2H_4Br_2$

STRUCTURAL FORMULA $BrCH_2CH_2Br$

PHYSICAL AND CHEMICAL PROPERTIES Colorless [118], colorless to pale yellow [144], liquid [53]. Molecular weight, 187.884. Melting point, 9.97°C [118], 9.3°C [179]. Boiling point, 131.5°C [179], 131.6°C [118]. Vapor pressure, 11 mm Hg (25°C). Specific gravity, 2.172 (25/25°C). [179] Refractive index, 1.53789 [118], 1.5357 (25°C) [53]. Soluble in alcohol, ether. Stable. [118]

TOXICITY Man. Probable LD, 50-500 mg/kg. Inhalation causes delayed pulmonary lesions. Death appears to be due to respiratory or circulatory failure, complicated by pulmonary edema. Fatal liver damage reported. [101] Liquid and vapor dangerous to eyes, cause inflammation of the conjunctiva. [250]

Animals.

Animal	LD_{50}, mg/kg	Route
Guinea pig	110(98-122)	p.o.
Mouse, ♀	420(353-500)	p.o.
Rat, ♀	117(108-126)	p.o.
Rat, ♂	146(126-170)	p.o.
Rabbit, ♀	55(44-69)	p.o.
Chicken	79(53-117)	p.o.

[47]

USE Agricultural.

79. ETHANE, 1,1,1-TRICHLORO-

ALTERNATIVE NAMES Methyl chloroform; 1,1,1-Trichloroethane.

MOLECULAR FORMULA $C_2H_3Cl_3$

STRUCTURAL FORMULA Cl_3CCH_3

79. ETHANE, 1,1,1-TRICHLORO- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [69,118]. Molecular weight, 133.415. Boiling point, 71-74.1°C [228], 72-76°C [69], 75°C [53]. Specific gravity, 1.3249 (26/4°C), 1.435 (25/25°C) [118]. Refractive index, 1.43765 (21°C) [118]. Soluble in ether. Insoluble in water. [228] Miscible with alcohol, benzene, carbon tetrachloride.

TOXICITY

Animal	MLD, mg/kg	Route	Time of Death
Dog	750[1]	p.o.	24 hr
Dog	95[1]	i.v.	30 min
Rabbit	500[1]	s.c.	24 hr

[120]

Animal	Dose	mg/L	ppm	Exposure Time
Mouse	MLC	65	11,000	2 hr
Rat	LC_{50}	97.9	18,000	3 hr
Rat	LC_{50}	82	14,000	7 hr

[120]

USE Protectant of materiel.

80. ETHANE, 1,1,2-TRICHLORO-

ALTERNATIVE NAMES 1,1,2-Trichloroethane; Vinyl trichloride.

MOLECULAR FORMULA $C_2H_3Cl_3$

STRUCTURAL FORMULA Cl_2CHCH_2Cl

PHYSICAL AND CHEMICAL PROPERTIES Colorless clear liquid. Sweet odor. Molecular weight, 133.415. Melting point, -36.7°C. Boiling point, 113.5°C [118]. Specific gravity, 1.4432, 1.438 (25/25°C). Refractive index, 1.4458 [53], 1.4711 [118]. Miscible with alcohol, benzene, ether, carbon tetrachloride, esters, ketones. Insoluble in water.

TESTS In vivo. Rhizopus nigricans Fr.: 2 varieties of peaches. With 1:10,000 concentration, severe injury to fruit; 1:20,000, no injury and Rhizopus was reduced 47%. [263]

Monilinia fructicola (Wint.) Honey, and Rhizopus nigricans Fr.: Peaches and plums inoculated artificially with a mixed spore suspension of the above organisms; incubated at 80°F and above 90% relative humidity for 24-hour period prior to treatment

/1/ In oil.

with compound. Fruit placed in closed glass containers, inside of which compound was introduced in open glass containers, permitting complete volatilization. After 24-hour treatment period, fruit was removed and stored at laboratory temperature at a relatively high humidity for an additional 72 hours. Rot completely inhibited; some browning of fruit at 1:4000, less browning at 1:10,000. [307]

Phomopsis citri, and Diplodia natalensis (stem-end rot in citrus fruit): 500 cc in 18 cubic feet. Excellent control; no injury to rind of fruit. [291]

TOXICITY Man. Locally irritating effect on mucous membranes, especially the eyes and nose. May cause corneal burns. Known to have harmful effect on the liver. [250]

Animals. Mice: Smallest lethal concentration, 1.2% by volume in air; 0.8% by volume in air caused complete narcosis. [250] LC_{50} in rats, approximately 2000 ppm for 4 hours. MLD in rabbits, 500 mg/kg, s.c. MLD in dogs, 750 mg/kg, p.o., in oil. [171]

USE Agricultural.

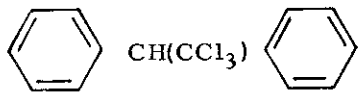
CAUTION Handlers should use protective equipment.

81. ETHANE, 1,1,1-TRICHLORO-2,2-DIPHENYL-

ALTERNATIVE NAMES 1-Trichloro-2,2-bis(phenyl)ethane; 1,1-Diphenyl-2,2,2-trichloroethane.

MOLECULAR FORMULA $C_{14}H_{11}Cl_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless crystals. Molecular weight, 285.599. Melting point, 60-62°C [85], 64°C [228], 66.5-67.5°C [288]. Soluble in common organic solvents. Insoluble in water. Stable in closed containers at room temperature.

TESTS In vitro. Aspergillus niger (Van Tiegham):

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	53	52	51	48	43
	55	54	54	52	48

81. ETHANE, 1,1,1-TRICHLORO-2,2-DIPHENYL- (Concluded)

TOXICITY Carassius auratus (goldfish): 1 fish per bowl of fresh water; exposure, 3 days. 4-10 ppm caused less than 100% mortality. Gambusia affinis (mosquito fish): Same test. MLD_{100}, approximately 2 ppm.

Mice: 250 mg/kg, i.p., daily for 5 days did not produce death. 500 mg/kg, i.p., daily for 5 days, resulted in death in 7 days. [261] Rat: 1000 mg/kg, s.t., non-toxic [296].

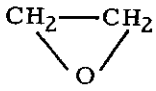
USE Protectant of materiel.

CAUTION Avoid prolonged breathing of vapors [85].

82. ETHYLENE OXIDE

ALTERNATIVE NAMES 1,2-Epoxyethane; Oxirane.

MOLECULAR FORMULA C_2H_4O

STRUCTURAL FORMULA 

PHYSICAL AND CHEMICAL PROPERTIES Mobile, colorless liquid at low temperatures, colorless gas at ordinary temperatures [53]. Molecular weight, 44.052. Melting point, -111.3°C. Boiling point, 10.73°C. [53] Vapor pressure, 1323 mm Hg (25°C), 1095 mm Hg (20°C) [180]. Specific gravity, 0.711 (20/20°C) [53], 0.89 (7/4°C) [118]. Soluble in common organic solvents. Miscible with water [118].

TOXICITY Man. Causes intolerable irritation to eyes and nose [180,250]. Intensely irritating to skin, mucous membranes and lungs; causes pulmonary edema. [101]

Animals. Guinea pigs: Nose and eye irritation; blood-tinged and frothy serous exudate from nostrils. Unsteadiness and staggering, inability to stand. Respiratory disturbances, dyspnea, death. [101]

Animal	Dose	mg/L	Exposure Time	Time of Death
Guinea pig	LC	9	1 hr	40 hr
Guinea pig	LC	36	1-½ hr	24 hr
Guinea pig	LC	90-180	Continuous	Few min
Rat	LC_{50}	7.2	4 hr	
Rat	LC	104	Continuous	6 hr
Rat	LC	180	39 min	24 hr
Rat	LC	450		Instant

[120]

82. ETHYLENE OXIDE (Concluded)

USE Protectant of materiel: textiles, paper [111]. Agricultural: stored food products [180].

CAUTION Individuals exposed to compound should wear chemical safety goggles and respirator [250]. Extremely flammable.

83. ETHYLENE, TETRACHLORO-

ALTERNATIVE NAMES Tetrachloroethylene; Perchloroethylene.

MOLECULAR FORMULA C_2Cl_4

STRUCTURAL FORMULA $Cl_2C=CCl_2$

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]. Ether-like odor [120]. Molecular weight, 165.848. Melting point, -22.18°C [118], -22.35°C [250]. Boiling point, 121.02°C [118], 121.20°C [250]. Specific gravity, 1.62272 [118], 1.611 (15/4°C) [250]. Refractive index, 1.50534. Insoluble in water. [118]

TESTS In vivo. Monilinia fructicola (Wint.) Honey, and Rhizopus stolonifer (Fr.) Lind.: Peaches inoculated with spore suspension in beef-peptone broth and 0.1% Tween 20; Monilinia sprayed on uninjured fruit, Rhizopus sprayed or dipped into shallow cut. Peaches individually wrapped in copper impregnated paper and kept at 75°F. Readings taken at 3 and 6 days.

Reading	Compound[1]	Organism	Reduction[2, 3]
3 da	Tetrachloroethylene	Monilinia	83-100
	Sulfur dust		61-70
	Tetrachloroethylene, plus sulfur dust		93
	Tetrachloroethylene	Rhizopus	71-79
	Sulfur dust		1-4
	Tetrachloroethylene, plus sulfur dust		74
6 da	Tetrachloroethylene	Monilinia	2-15
	Sulfur dust		48-52
	Tetrachloroethylene, plus sulfur dust		70
	Tetrachloroethylene	Rhizopus	55-61
	Sulfur dust		-1 to +7
	Tetrachloroethylene, plus sulfur dust		51

[264]

/1/ Tetrachloroethylene, 1:20,000; sulfur dust, 94%; tetrachloroethylene, plus sulfur dust, 1:20,000. /2/ Reduction as percentage of decay in untreated fruit. /3/ Minus sign indicates increased decay.

83. ETHYLENE, TETRACHLORO- (Concluded)

TOXICITY Man. Maximum safe concentration, 100 ppm. Slight irritation of mucous membranes, skin and cornea; liver and kidney damage; moderate narcotic effect. [71]

Animals. Cat exposed to 3½% by volume in air developed light narcosis in 23 minutes, and deep narcosis in 40 minutes [250].

Animal	Dose	mg/kg	Route	Time of Death
Cat	LD	6496	p.o.	6-36 hr
Dog	MLD	85[1]	i.v.	30 min
Dog	LD	6,496-24,360	p.o.	7½-72 hr
Mouse	LD_{50}	8850[2]	p.o.	
Mouse	LD_{50}	10,900[1]	p.o.	
Mouse	LD	8120	p.o.	2-9 hr
Rabbit	MLD	2200	s.c.	24 hr
Rabbit	LD	8120	p.o.	7-20 hr

[120]

COMPARATIVE TOXICOLOGY Least toxic of the chlorinated hydrocarbons [154].

USE Agricultural.

CAUTION Use of a respirator recommended [250].

84. ETHYLENE, TRICHLORO-

ALTERNATIVE NAMES Trichloroethylene; Ethinyltrichloride.

MOLECULAR FORMULA C_2HCl_3

STRUCTURAL FORMULA $Cl_2C{=}CHCl$

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]. Mild, chloroform-like odor [250]. Molecular weight, 131.399. Melting point, -73°C [118]. Boiling point, 87°C [118], 88°C [71]. Vapor pressure, 60 mm Hg (20°C). Specific gravity, 1.45560 (25/4°C) [118]. Refractive index, 1.4735. Miscible with all common organic solvents. Practically insoluble in water. [53]

/1/ In oil. /2/ Chemically pure.

TESTS In vivo. Monilinia fructicola (Wint.) Honey, and Rhizopus stolonifer (Fr.) Lind.: Peaches inoculated with spore suspension in beef-peptone broth and 0.1% Tween 20; Monilinia sprayed on uninjured fruit, Rhizopus sprayed or dipped into shallow cut. Peaches individually wrapped in copper impregnated paper and kept at 75°F. Readings taken at 3 and 6 days.

Reading	Compound[1]	Organism	Reduction[2,3]
3 da	Trichloroethylene	Monilinia	91-97
	Sulfur dust		61-70
	Trichloroethylene	Rhizopus	79-82
	Sulfur dust		1-4
6 da	Trichloroethylene	Monilinia	-5 to -14
	Sulfur dust		48-52
	Trichloroethylene	Rhizopus	59
	Sulfur dust		-1 to + 7

[264]

TOXICITY Man. Probable LD, 50-500 mg/kg[101]. Strong narcotic action [154]. Toxic when inhaled or with prolonged or repeated contact with skin or mucous membranes; toxic when ingested. Lacrimation, burning of the eyes, irritation of nose and throat, nausea, vomiting, drowsiness, attitude of irresponsibility; even an appearance resembling intoxication. [250] 5 deaths reported, 4 from exposure to high vapor concentrations, 1 from presence of compound in beverage [171].

Animals. Rats (200 ppm), rabbits (200 ppm), guinea pigs (100 ppm), and monkeys (400 ppm) exposed 7 hours daily, 5 days weekly for 6 months, showed no adverse effects [171].

Animal	Dose	mg/kg	Route	Time of Death	Reference
Cat	LD	5864	p.o.		120
Dog	MLD	150	i.v.	30 min	120
Dog	LD	5864	p.o.		120
Dog	LD	150	s.c.		47
Rabbit	MLD	1800[4]	s.c.	24 hr	120
Rabbit	LD	7330	p.o.		120

Animal	Dose	mg/L	ppm	Exposure Time	Time of Death
Guinea pig, young	LC	200	37,200	Continuous	9-12 min
Guinea pig, adult	LC	200	37,200	Continuous	40 min
Mouse	MLC	42	7800	2 hr	
Rabbit	LC	107.6	20,000	Continuous	2 hr

[120]

/1/ Trichloroethylene, 1:20,000; sulfur dust, 94%. /2/ Reduction as percentage of decay in untreated fruit. /3/ Minus sign indicates increased decay. /4/ In oil.

84. ETHYLENE, TRICHLORO- (Concluded)

USE Agricultural.

CAUTION Handlers should use protective equipment [250].

85. FILIPIN

SOURCE Streptomyces filipinensis.

MOLECULAR FORMULA $C_{30}H_{50}O_{10}$

PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals [108]; fine feathery needles [121]. 2 allotropic forms, transition occurring at 147°C. Melting point, 195-205°C. Soluble in methanol, ethanol, pyridine, glacial acetic acid. Insoluble in water. Thermolabile. Susceptible to autoxidation, especially in light. Stable in dark in air under refrigerated conditions; stable in dilute ethanolic solution (50 μg/ml), but unstable at 10 mg/ml under all conditions. Deteriorates slowly in methanolic solution at pH 2 and 11. [121]

TESTS In vitro. Minimum inhibitory concentration (μg/ml):

	Incubation Time		
	48 hr	72 hr	96 hr
Aspergillus niger		3.9	31.0
Blastomyces dermatitidis	31.0		
Candida albicans	7.7		
Coccidioides immitis	15.0		
Colletotrichum lindemuthianum		1.9	3.9
Cryptococcus neoformans	0.95		
Dendrophoma obscurans		7.8	7.8
Diplodia sp		31.0	1000.0
Endothia parasitica		1.9	1.9
Fusarium oxysporum dianthi		7.8	15.0
Geotrichum sp	31.0		
Gnomonia fragariae Kleb.		0.95	0.95
Helminthosporium sativum		7.8	7.8
Histoplasma capsulatum	7.7		
Hormodendrum compactum	15.5		
Microsporum audouini Gruby	7.7		
Monosporium apiospermum	7.7		
Nocardia asteroides	31.0		
Penicillium digitatum		3.9	7.8
P. notatum		31.0	62.0
Phialophora verrucosa	15.5		
Phoma betae Fr.		3.9	7.8
Phomopsis sp		3.9	7.8

(continued)

85. FILIPIN (Concluded)

	Incubation Time		
	48 hr	72 hr	96 hr
Rhizoctonia solani		500.0	500.0
Sclerotinia sclerotiorum		7.8	15.0
Sporotrichum schenckii	7.7		
Thielaviopsis sp		3.9	3.9
Trichophyton rubrum	7.7		

[121]

In vivo. Sprays with crude filipin partially protected young tomato plants from gray leaf spot caused by Stemphylium solani [108].

PHYTOTOXICITY Very slight, even from spray of 1000 μg/ml [108]. Concentration of 100 μg/ml had no deleterious effect on the germination of pea and tomato seeds [121].

USE Medicinal; agricultural.

86. FORMIC ACID

ALTERNATIVE NAME Methanoic acid.

MOLECULAR FORMULA CH_2O_2

STRUCTURAL FORMULA HCOOH

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid. Pungent, penetrating odor. [53] Molecular weight, 46.026. Melting point, 8.3°C [53], 8.4°C [118]. Boiling point, 100.8°C [53]; 107°C [118]. Specific gravity, 1.2178 [53], 1.22647 (15/4°C) [118]. Refractive index, 1.37137. Soluble in water, alcohol, ether [53]; glycerin [118].

TOXICITY Man. Dangerously caustic, corrosive [53]. Highly irritating to skin, eyes, and mucous membranes [250].

Animals.

Animal	MLD, mg/kg	Route
Dog	4000 (Na salt)	p.o.
Dog	3000 (Na salt)	i.v. (slow injection)
Rabbit	239	i.v.

[120]

COMPARATIVE TOXICOLOGY More irritating than acetic acid [250].

USE Protectant of materiel.

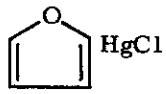
CAUTION Store in cool, well-ventilated place, away from areas of acute fire hazard and powerful oxidizing agents [250]. In handling, avoid breathing vapor [53]; wear chemical safety goggles and respirator, and, with high concentrations, protective clothing [250].

87. FURAN, 2-(CHLOROMERCURI)-

ALTERNATIVE NAME Mercury, 2-furyl-chloride.

MOLECULAR FORMULA C_4H_3ClHgO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [118], white [281], crystalline powder [118]. Molecular weight, 303.131. Melting point, 148°C [118], 151-152.5°C [281]. Soluble in hot alcohol [118], acetone, dioxane [281]. Slightly soluble in ether [118]. Insoluble in water, diphenyl ether, alcohol, chloroform [281]. Slight darkening on heating [118].

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

ppm	% Inhibition
250	100
150	100
125	100
75	100
37.5	100

[281]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, strain 640: Melted agar seeded with conidia of the fungus was hardened and a small portion of the chemical placed on the plate in a 3-5 mm area. If liquid, chemical was placed in a glass cylinder. Plates were incubated at 30°C and the zone of inhibition read at 1- and 2-week intervals. Untreated controls were incubated under the same conditions. Width of the zone of inhibition measured not only fungicidal action but also the diffusability of the material through the agar. Radius of inhibition zone, 1.0 cm. [281]

TOXICITY Man. Undiluted compound causes some reddening of skin. Alcohol solutions cause blistering. [281]

Animals. Mice: Compound dissolved in water or propylene glycol and administered i.p.; 10-day observation period.

mg/kg	Mortality
10	0/4
20	2/8
40	10/10

[280]

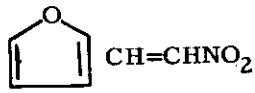
USE Protectant of materiel.

88. FURAN, 2-(2-NITROVINYL)-

ALTERNATIVE NAME Ethylene, 1-(2-furyl)-2-nitro-.

MOLECULAR FORMULA $C_6H_5NO_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals. Molecular weight, 139.108. Melting point, 74-75°C. [281] Boiling point, 110°C (10 mm Hg) [281]; decomposes, 120°C [228]. Specific gravity, 1.442. Vapor pressure, 0.014 mm Hg (20°C), 0.023 mm Hg (25°C), 0.036 mm Hg (30°C). Soluble in benzene, methanol. Less soluble in carbon tetrachloride, petroleum ether. [281]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound, inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

ppm	% Inhibition
250	100
150	100
125	100
75	100
37.5	100

[281]

10-fold dilutions of test compound added to spores in depression slide cavity. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: Complete kill, 1000 ppm. [281]

USE Protectant of materiel.

89. GLUTARIMIDE, 3-[2-(3,5-DIMETHYL-2-OXOCYCLOHEXYL)-2-HYDROXYETHYL]-

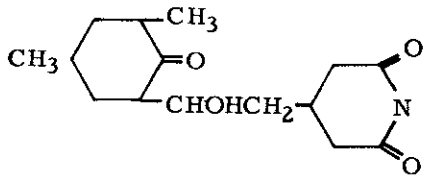
ALTERNATIVE NAMES Cycloheximide; Actidione.

SOURCE Streptomyces griseus.

MOLECULAR FORMULA $C_{15}H_{23}NO_4$

89. GLUTARIMIDE, 3-[2-(3,5-DIMETHYL-2-OXOCYCLOHEXYL)-2-HYDROXYETHYL]- (Continued)

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless plates [121]. Molecular weight, 281.342. Melting point, 115-116.5 [121]. Very soluble in chloroform, methanol, acetone [53]. Soluble in water, all organic solvents except saturated hydrocarbons [121]. Moderately soluble in 99% isopropyl alcohol, n-butanol, amyl acetate. Very slightly soluble in carbon tetrachloride, saturated hydrocarbons. Stable at pH 3-5 for several weeks. Rapidly destroyed in alkaline solution. [53]

TESTS In vitro. Alternaria spp, Aspergillus spp, Fusarium spp, Hormodendrum spp: 0.1 μg/ml water inhibited growth 90-100%. Neurospora spp, Penicillium spp, Rhizopus spp, Saccharomyces spp: 0.1 μg/ml water inhibited growth 98-100% [233].

Poria microspora: Growth completely inhibited on media containing 210 ppm. (Better effect obtained with synthetic broth than with highly organic media.) [158]

Nocardia asteroides, 2 strains: Sabouraud's agar; incubated 6-8 days at 38°C. 20-100 μg/ml partially inhibited growth. [271]

Stemphylium sarcinaeforme Cav.: MED, 10 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 1 ppm. [55]

Cryptococcus neoformans, Aspergillus niger, Saccharomyces cerevisiae: Growth inhibited at 0.2-50 μg/ml. Most fungal animal pathogens not susceptible (>1000 μg/ml): Candida albicans, Blastomyces dermatitidis, Epidermophyton floccosum, Hormodendrum pedrosoi, Nocardia asteroides, Trichophyton spp. Phytopathogenic fungi inhibited by 5 μg/ml, or less: Cladosporium fulvum, Colletotrichum lagenarium, Diaporthe citri, Diplocarpon rosae, Diplodia zeae, Endothia parasitica, Heterosporium iridis, Physalospora tucumanensis, Sclerotinia fructicola, Sclerotium rolfsii, Ustilago tritici, U. zeae, Venturia inequaelis. [121]

In vivo. Sclerotinia homeocarpa (dollar spot on bent grass strains): Compound sprayed on golf greens at 2-week intervals. 200 ppm gave effective control. [308]

S. fructicola: 50-100 ppm gave peaches good protection [121].

Erysiphe polygoni D.C. (mildew on red kidney bean): Plant sprayed prophylactically when 10-12 days old and at 6-10 day intervals thereafter. Lifetime protection at 1, $2\frac{1}{2}$, 5, and $7\frac{1}{2}$ ppm. At concentrations greater than 100 ppm, evidence of toxicity in young plants. [90]

89. GLUTARIMIDE, 3-[2-(3,5-DIMETHYL-2-OXOCYCLOHEXYL)-2-HYDROXYETHYL]- (Concluded)

TOXICITY Man. Highly toxic [101]. Potent skin irritant [53]. Crude preparations highly irritating to skin [121].

Animals. Evidence of cumulative toxicity with repeated i.p. injections of sublethal doses [241]. Rats, dogs, and monkeys exhibited excessive salivation, diarrhea, blood-stained feces [101]. Oral doses as low as 1 mg/kg fatal to rats. Rabbits tolerated approximately 4.5 mg/kg, p.o. [121]

Animal	LD_{50}, mg/kg	Route	Reference
Guinea pig	65	p.o.	180
Monkey	60	p.o.	180
Mouse	133	p.o.	180
Mouse	150	i.v.	121
Rat	1	p.o.	120, 180
Rat	2.5	p.o.	180
Rat	2.5	i.v.	121
Rat	2.7	s.c.	121

PHYTOTOXICITY Toxic action in some plants (peach, tomato, bean, geranium) limits use as agricultural fungicide. 100 μg/ml induced specific aberrations in mitotic behavior of onion root cells. 10-50 ppm inhibited Ascochyta pisi infection in peas, but was toxic to pea seeds. [121]

USE Protectant of materiel; medicinal; agricultural.

90. HIPPURIC ACID

ALTERNATIVE NAMES N-Benzoylglycine; Benzamidoacetic acid.

MOLECULAR FORMULA $C_9H_9NO_3$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES Colorless crystals. Molecular weight, 179.170. Melting point, 187-188°C [283], 187-190.2°C [228]; decomposes with further heating [53]. Specific gravity, 1.371 [118,283]. Refractive index, 1.535 [118]. Soluble in hot water, alcohol, ether [53]. Slightly soluble in chloroform [228], acetone [283]. Insoluble in carbon disulfide [228]; petroleum ether, benzene [283].

90. HIPPURIC ACID (Concluded)

TESTS In vitro. 10-fold dilutions of compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 1000 ppm. [55]

Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 12% [228].

TOXICITY Animals. Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight, exposure 24 hours. No injury. [291]

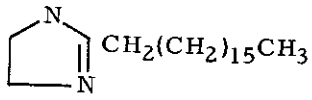
USE Protectant of materiel.

91. 2-IMIDAZOLINE, 2-HEPTADECYL-

ALTERNATIVE NAMES 2-Heptadecylglyoxalidine; Glyoxalidine.

MOLECULAR FORMULA $C_{20}H_{40}N_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Crystalline solid [56]; waxy, solid grease [144]. Molecular weight, 308.536. Melting point, 85°C [179]. Boiling point, 200°C (2 mm Hg). Slightly soluble in water. Soluble in alcohol, benzene. [53] Stable [56].

TOXICITY Man. Poorly absorbed except in presence of solvents. May cause opaque cornea, keratoconus, extensive necrosis [250]. Concentrated forms irritating and sensitizing to skin. [56]

Animals. Toxicity in animals relatively low [95]. Congestion and petechial hemorrhage of lungs, congestion of liver and kidneys, varying degrees of minor gastrointestinal irritation. Rats developed diarrhea, redness of mouth and nose, often hematoporphyria about eyes and nose after oral administration. LD_{50} in rats, 1.3 g/kg, p.o. (10% suspension). Guinea pigs on 0.15% and 0.03% in dry diet for 1 year showed no deleterious effects. Dogs tolerated 0.07% in dry diet. [36]

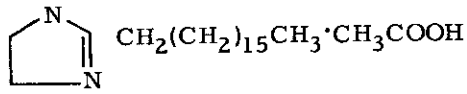
USE Agricultural: foliage application [179, 316]; fruits and ornamentals [56]; particularly effective against cherry leaf spot, apple scab [95].

CAUTION Handlers should wear chemical safety goggles [250].

92. 2-IMIDAZOLINE, 2-HEPTADECYL-, ACETATE

ALTERNATIVE NAMES 2-Heptadecyl-2-imidazoline acetate; 2-Heptadecylglyoxalidine acetate.

MOLECULAR FORMULA $C_{20}H_{40}N_2 \cdot C_2H_4O_2$

STRUCTURAL FORMULA  $CH_2(CH_2)_{15}CH_3 \cdot CH_3COOH$

PHYSICAL AND CHEMICAL PROPERTIES Light orange crystals [53,205]; waxy solid [92]. Slight odor [205]. Molecular weight, 368.588. Melting point, 62-68°C. Specific gravity, 1.035 (20°C) [180]. Soluble in isopropanol, 39%. Partially soluble in propylene glycol, ethylene dichloride. Insoluble in water, acetone, toluene. [205]

TOXICITY Man. Low toxicity [180]. Concentrated solutions irritating to skin [101].

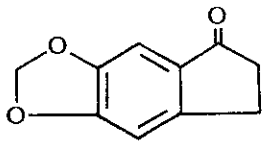
Animals. LD_{50} in rats, 1.34 g/kg, p.o. 2 g/kg, applied to skin of rabbits as a 4% solution in benzene, resulted in no fatalities but caused skin necrosis. Rabbit belly vesicant test: 10% in benzene caused edema, 1% caused erythema; 10% in ethanol caused erythema. 1% of test compound in propylene glycol injurious to eyes of rabbits. [205]

USE Protectant of materiel. Agricultural: foliage protectant [180].

93. 5H-INDENO[5,6]-1,3-DIOXOL-5-ONE, 6,7-DIHYDRO-

ALTERNATIVE NAME 5,6-Methylenedioxy-hydrindone-1.

MOLECULAR FORMULA $C_{10}H_8O_3$

STRUCTURAL FORMULA 

PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 176.164.

TESTS In vitro. Stemphylium sarcinaeforme Cav.:

µg/sq cm	% Inhibition
1000	100
100	100
10	100
1	0

[55]

93. 5H-INDENO[5,6]-1,3-DIOXOL-5-ONE, 6,7-DIHYDRO- (Concluded)

Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm did not inhibit spore germination [55].

TOXICITY Mice (Banks strain, female) survived 500 mg/kg, i.p., in ½% carboxy methyl cellulose, isotonic saline solution [260].

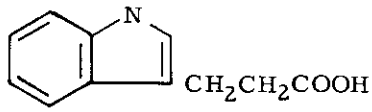
USE Agricultural.

94. 3-INDOLEPROPIONIC ACID

ALTERNATIVE NAME β-(Indole-3)-propionic acid.

MOLECULAR FORMULA $C_{11}H_{11}NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Tan to brown powder [69]. Molecular weight, 189.206. Melting point, 132.5-133.5°C [288], 132.8-133.7°C [69]. Soluble in alcohol, ether [69].

TESTS In vitro. Aspergillus niger (Van Tiegham): 1 drop of spore suspension and 250 ppm of test compound in nutrient-toxic-agar; incubated 96 hours at 30°C. Growth inhibited 83%. [291]

TOXICITY Animals. Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight, exposure 24 hours. No injury. [261]

Mice survived 15.7-500 mg/kg, i.p. [261]

USE Protectant of materiel.

95. IODINE

MOLECULAR FORMULA I_2

PHYSICAL AND CHEMICAL PROPERTIES Black lustrous crystals. Molecular weight, 253.82. Vapor pressure, 0.030 mm Hg (0°C), 0.469 mm Hg (30°C). Soluble in chloroform, ether, glacial acetic acid. Freely soluble in solution of hydriodic acid or iodides.

TESTS In vitro. Organisms susceptible: Candida albicans, Sporotrichum schenckii, Epidermophyton floccosum (Harz) Langeron and Milochevitch, Microsporum audouini Gruby, M. canis Bodin, M. gypseum (Bodin) Guiart and Grigorakis, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, T. (purpureum) rubrum (Castellani) Sabouraud [222].

TOXICITY Man. Extremely toxic. Probable LD, 5-50 mg/kg. [101] Pain in the throat and stomach, vomiting, purging and intense thirst; giddiness, faintness and convulsions.

Animals. MLD in rabbits, 175-180 mg/kg, s.c. LD in dogs, 40 mg/kg, i.v. [120]

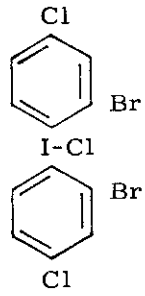
USE Medical: systemic mycoses.

96. IODONIUM CHLORIDE, BIS(2-BROMO-4-CHLOROPHENYL)-

ALTERNATIVE NAME Bis(2,4-bromochlorophenyl)iodonium chloride.

MOLECULAR FORMULA $C_{12}H_6Br_2Cl_2I^+ \cdot Cl^-$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White solid [17]. Molecular weight, 563.281. Stable [17].

96. IODONIUM CHLORIDE, BIS(2-BROMO-4-CHLOROPHENYL)- (Concluded)

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound, inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C; terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	100

250 ppm inhibited growth 100%. [17]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [17]

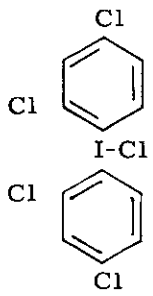
USE Protectant of materiel.

97. IODONIUM CHLORIDE, BIS(2,4-DICHLOROPHENYL)-

ALTERNATIVE NAME Bis(2,4-dichlorophenyl)iodonium chloride.

MOLECULAR FORMULA $C_{12}H_6Cl_4I^+ \cdot Cl^-$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White [17] solid [228]. Molecular weight, 454.363. Stable [17].

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound, inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours; results reported as % inhibition of growth compared to normal controls.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	100

97. IODONIUM CHLORIDE, BIS(2,4-DICHLOROPHENYL)- (Concluded)

250 ppm inhibited growth 100%. [17]

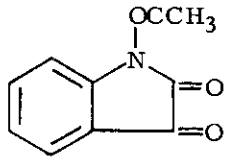
USE Protectant of materiel.

98. ISATIN, 1-ACETYL-

ALTERNATIVE NAME Pseudoisatin, 1-acetyl-.

MOLECULAR FORMULA $C_{10}H_7NO_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow needles. Molecular weight, 189.164. Melting point, 141°C. Soluble in alcohol, benzene. [118]

TESTS In vitro. 10-fold dilutions of test compound added to spore suspension in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 1000 ppm. [55]

Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 3% [228].

TOXICITY Mice tolerated 500 mg/kg, i.p. [264], and rats 500 mg/kg, s.t. [148].

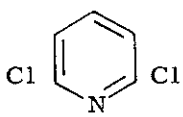
USE Protectant of materiel.

99. ISONICOTINIC ACID, 2,6-DICHLORO-

ALTERNATIVE NAME 2,6-Dichloroisonicotinic acid.

MOLECULAR FORMULA $C_6H_3Cl_2NO_2$

STRUCTURAL FORMULA



99. ISONICOTINIC ACID, 2,6-DICHLORO- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Buff-colored crystals. Molecular weight, 192.006. Melting point, 210°C. Soluble in ethyl alcohol, dilute alkali. Insoluble in water. Fairly stable.

TESTS In vitro.

	µg/sq cm	% Inhibition
Stemphylium sarcinaeforme Cav.	1000	100
	100	100
	10	100
	1	0
Sclerotinia fructicola (Wint.) Rehm.	1000	100
	100	100
	10	0

[55]

USE Agricultural.

100. ISOTHIOCYANIC ACID, ALLYL ESTER

ALTERNATIVE NAMES Allyl mustard oil; 2-Propenyl isothiocyanate.

MOLECULAR FORMULA C_4H_5NS

STRUCTURAL FORMULA $CH_2{=}CHCH_2NCS$

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]; turns yellow [250]. Irritating odor [192]. Molecular weight, 99.154. Melting point, -100°C [118]. Boiling point, 150.7°C [118], 150.9 ± 0.1 [228]. Specific gravity, 1.0126 [228], 1.0155 (15/4°C) [118]. Refractive index, 1.5266 [228], 1.52212 (24°C) [118]. Slightly soluble in water; miscible with alcohol and most organic solvents [192].

TOXICITY Man. Very irritating to lungs, eyes, skin [250]. A violent irritant unless diluted; aqueous solutions more irritating than oil solutions. [101]

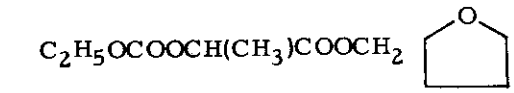
USE Protectant of materiel. Agricultural: mold preventive for fodder [118].

101. LACTIC ACID, ETHYL CARBONATE, TETRAHYDROFURFURYL ESTER

ALTERNATIVE NAME Ethyl 1-carbotetrahydrofurfuryloxyethyl carbonate.

MOLECULAR FORMULA $C_{11}H_{18}O_6$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Liquid [81]. Molecular weight, 246.254. Boiling point, 110°C (0.8 mm Hg). Specific gravity, 1.1392. Refractive index, 1.4433. [81]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	4	4	0	0	0

250 ppm inhibited growth 100%. [81]

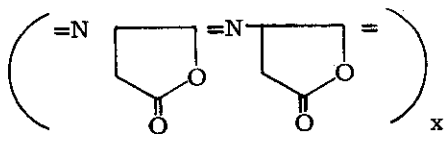
10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm. [81]

USE Protectant of materiel.

102. MALEAMIC ACID[1]

MOLECULAR FORMULA $(C_4H_3NO_2)_x$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Decomposes, 300°C. Soluble in phenol, glycol, polyhydric alcohols. Slightly soluble in water. Insoluble in ether, hydrocarbons, monohydric aliphatic alcohols. Stable. [18]

/1/ Peptide condensation product.

102. MALEAMIC ACID (Concluded)

TESTS In vitro. 10-fold dilutions from 10,000 to 10 ppm. Compound added to spore suspension in depression slide, incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm. [55]

Aspergillus niger: 250 ppm inhibited growth 8% [228].

TOXICITY Animals. Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm; exposure 24 hours. No injury. [297]

Mice: 125 mg/kg/da, i.p. for 5 days, tolerated; 250 mg/kg/da, i.p. for 5 days, resulted in death. [261]

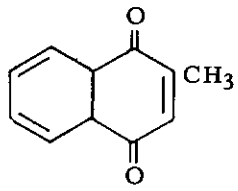
USE Protectant of materiel.

103. MENADIONE

ALTERNATIVE NAMES Vitamin K_3; Menaphthone; Menaphthene; Aquinone; Aquakay; Kappakin; Davitamon K; Hemodal; Kaergona; Kapilin; Kapilon; Kappaxan; Kareon; Kaviton; Kayquinone; Kolklot; Synkay; Menaquinone; Thyloquinone; 1,4-Naphthoquinone, 2-methyl-.

MOLECULAR FORMULA $C_{11}H_8O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow, crystalline powder. Nearly odorless. [8] Molecular weight, 172.174. Melting point, 105-107°C. Soluble in alcohol, benzene, vegetable oils. Moderately soluble in chloroform, carbon tetrachloride. Insoluble in water. Affected by sunlight. [53]

TESTS In vitro. Alternaria solani (Ell. and Mart.) J. and G., and Sclerotinia fructicola (Wint.) Rehm.: Standard screening test procedure adopted by American Phytopathological Society. 0.01-1 ppm of test compound inhibited spore germination 50% (LD_{50}). [189]

In vivo. Alternaria solani (Ell. and Mart.) J. and G.: Foliage spray controlled infection in tomato plants. ED_{95}, 2000 ppm. [189]

TOXICITY Man. Irritating to respiratory tract and to the skin. Alcoholic solution has vesicant properties. [53]

103. MENADIONE (Concluded)

Animal	Dose	mg/kg	Route	Reference
Mouse	LD_{50}	41	i.p.	47
Mouse	LD_{100}	1000[1]	p.o.	120
Mouse	LD_{100}	200[1]	i.p.	120
Chicken	LD_{100}	250[1]	i.p.	120

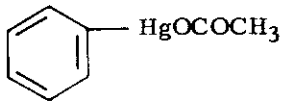
USE Medicinal.

104. MERCURY ACETATE, PHENYL-

ALTERNATIVE NAME Phenylmercuric acetate.

MOLECULAR FORMULA $C_8H_8HgO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless to light cream [157], small lustrous rhombic prisms [53, 318]. Odorless [318]. Molecular weight, 336.754. Melting point, 149-153°C [180], 148-150°C [318]. Vapor pressure negligible at room temperature. Soluble (g/100 g solvent) in water, 0.47; boiling water, 2.9; acetic acid (10%), 0.47; benzene, 1.8; "Carbitol," 11.8; ethyl alcohol, 5.2; sodium hydroxide (2%), 1.10 [53]. Stable to within a few degrees of melting point. Stable in neutral media. [318]

TESTS In vitro. Organisms susceptible: Epidermophyton floccosum (Harz) Langeron and Milochevitch, Microsporum audouini Gruby, M. canis Bodin, M. gypseum (Bodin) Guiart and Grigorakis, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, T. (purpureum) rubrum (Castellani) Sabouraud, T. (Achorion) schoenleinii (Lebert) Langeron and Milochevitch, T. tonsurans, T. (Achorion) violaceum Sabouraud [70].

In vivo. Sclerotinia laxa: Detached almond twigs, at flowering stage and bearing sporodochia, sprayed with test compound; kept in moist chamber 3-8 days. Conidia separated by crushing; plated, and incubated. No significant mortality with 0.05% and 0.1% solutions. [323]

/1/ Suspension in oil.

104. MERCURY ACETATE, PHENYL- (Concluded)

TOXICITY Man. Highly toxic [95, 180]. Classed as a primary irritant [42, 298]. Dust or strong solution causes skin blistering [53]. Repeated use may produce poisoning [70].

Animals. Mice: 15.6 mg/kg, i.p., daily for 5 days, non-lethal. 31.25 mg/kg resulted in death in 4-5 hours. [261]

COMPARATIVE TOXICOLOGY In tests on leather, compound more effective than phenyl mercuric nitrate [314].

USE Protectant of materiel: paint, paper, plastics, textiles, leather [111, 314]. Medicinal: dermatomycoses [70]. Agricultural: turf fungus diseases, apple scab [314].

105. MERCURY (II) CHLORIDE

ALTERNATIVE NAMES Bichloride of mercury; Mercury perchloride; Mercuric chloride.

MOLECULAR FORMULA $HgCl_2$

PHYSICAL AND CHEMICAL PROPERTIES White crystals or powder [53]. Molecular weight, 271.524. Melting point, 276°C [118], 277°C [92]. Boiling point, 302°C [118]. Slightly volatile at ordinary temperatures, appreciably so at 100°C [192]. Specific gravity, 5.44 (25°C) [118]. Soluble in water, alcohol, ether, pyridine, ethyl acetate [53]. Unstable in presence of alkalies, which precipitate mercuric oxychloride. Decomposes in presence of organic matter in sunlight. [180]

TESTS In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 1:4000 solution of test compound; dried, and stored for 3 weeks at 70°F. Decay prevented; no rind injury. [291]

TOXICITY Highly toxic [101, 180]. Corrosive to mucous membranes; severe nausea, vomiting, abdominal pain, diarrhea, kidney damage, prostration [192].

Animal	Dose	mg/kg	Route	Time of Death
Mouse	LD_{50}	23	s.c.	
Mouse	LD_{50}	7.6	i.v.	
Mouse	LD_{50}	14 ± 2.4[1]	i.v.	3 hr
Mouse	LD_{50}	4.8 ± 0.8[1]	i.v.	4 da
Rabbit	LD	10[2]	s.c.	
Rat	LD_{50}	37[3]	p.o.	

[120]

/1/ As mercury. /2/ In water. /3/ Approximately.

105. MERCURY (II) CHLORIDE (Concluded)

PHYTOTOXICITY Highly toxic to plants [180].

USE Protectant of materiel: paper, wood [53, 111, 192]. Agricultural: control of Fusarium spp [92].

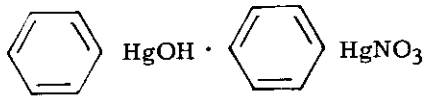
CAUTION Handle with extreme caution. Do not use on or near any food product. [96]

106. MERCURY NITRATE, PHENYL-

ALTERNATIVE NAME Phenylmercuric nitrate.

MOLECULAR FORMULA $C_6H_5HgNO_3 \cdot C_6H_6HgO$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Fine white crystals, or grayish powder [53]. Molecular weight, 634.436. Melting point, 175-185°C, with decomposition. Moderately soluble in glycerin. Slightly soluble in alcohol. Very slightly soluble in water. Insoluble in ether. [53]

TESTS In vitro. Organisms susceptible: Epidermophyton floccosum (Harz) Langeron and Milochevitch, Microsporum audouini Gruby, M. canis Bodin, M. gypseum (Bodin) Guiart and Grigorakis, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, T. (purpureum) rubrum (Castellani) Sabouraud, T. (Achorion) schoenleinii (Lebert) Langeron and Milochevitch, T. verrucosum, T. (Achorion) violaceum Sabouraud. [222]

TOXICITY Man. Dust or strong solution causes skin blistering [53]. Poisoning may result from continued use [222].

Animals.

Animal	LD_{50}, mg/kg	Route
Mouse	45	s.c.
Mouse	27	i.v.
Rat	63	s.c.

[120]

USE Protectant of materiel: mildew-proofing agent.

107. MERCURY OLEATE, PHENYL-

ALTERNATIVE NAME Phenylmercuric oleate.

MOLECULAR FORMULA $C_{24}H_{38}HgO_2$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES Amorphous solid. Oleo-resinous odor. [318] Molecular weight, 559.154. Decomposition starts at approximately 212°F. Non-volatile up to approximately 275°F. Soluble in most hydrocarbon solvents. Insoluble in water. Stable to ultraviolet light. [318]

TESTS In vivo. Chaetomium globosum, and Myrothecium verrucaria (Metarrhizium glutinosum) inhibited [111].

TOXICITY Six out of six rats survived 10 treatments of 27 mg/kg/da, p.o., but showed marked discomfort and weight loss. Autopsy, 14 days after treatments had ceased, revealed kidneys enlarged and slightly mottled. [78]

USE Protectant of materiel: textiles, paint [111]; wood [53].

108. METHANE, BROMO-

ALTERNATIVE NAMES Bromomethane; Methyl bromide; Monobromomethane.

MOLECULAR FORMULA CH_3Br

STRUCTURAL FORMULA CH_3Br

PHYSICAL AND CHEMICAL PROPERTIES Colorless, transparent, easily liquified gas, or volatile liquid. Burning taste. Chloroform-like odor. [53] Molecular weight, 94.950. Melting point, -84°C [53], -93.66°C [118]. Boiling point, 4.6°C [53], 3.56°C [118]. Vapor pressure, 1250 mm Hg (20°C). Specific gravity, 1.732 (0°C). Miscible with most organic solvents. [53]

TOXICITY Man. Vapors extremely hazardous [190]. Safe upper limit set at 17 ppm, above which respirators should be worn [180]. Injurious to nervous and cardiovascular systems, lungs. Contact severely burns skin, mucous membranes. Causes excessive fatigue, headache, nausea, vomiting, disturbances of hearing and vision, mental confusion, muscular weakness and collapse. Later there may be local or generalized infection, disturbances of sensations in the extremities, psychic abnormalities; respiration may be seriously affected and circulatory collapse may occur. [250]

108. METHANE, BROMO- (Concluded)

Animals.

Animal	LC_{100}, mg/L	ppm	Exposure Time	Time of Death
Rabbit	10	2570	Continuous	132 min
Rabbit	20	5140	Continuous	84 min
Rabbit	50	12,850	Continuous	30 min
Rat	0.63	514	Continuous	6 hr
Rat	10	2570	Continuous	42 min
Rat	0.84	5140	Continuous	24 min
Rat	50	12,850	Continuous	6 min

[120]

USE Agricultural [180].

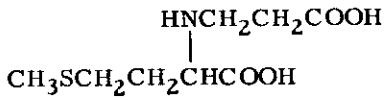
CAUTION Handlers should wear gloves made of plastic or canvas, high safety shoes and outer clothing of wool; gas-tight safety chemical goggles and respirator recommended. [250]

109. DL-METHIONINE, N-(2-CARBOXYETHYL)-

ALTERNATIVE NAME N-(β-Propionic acid)-DL-methionine.

MOLECULAR FORMULA $C_8H_{15}NO_4S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 221.274. Melting point, 212-215°C, with decomposition.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm inhibited spore germination. Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm did not inhibit spore germination. [55]

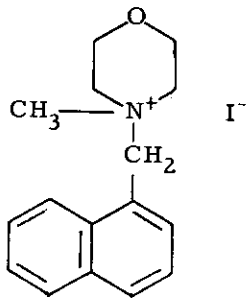
TOXICITY Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight; exposure 24 hours. No injury. [297]

USE Medicinal.

110. MORPHOLINIUM IODIDE, 4-METHYL-4-(1-NAPHTHYLMETHYL)-

MOLECULAR FORMULA $C_{16}H_{20}NO^{+}\cdot I^{-}$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 369.238. Melting point, 200°C.

TESTS In vitro. Sporotrichum schenckii: 3×10^7 spore concentration seeded to North's gelatine agar; treated with 3.0, 1.0, and 0.3% of test compound; incubated for 24 hours at 37°C.

Test Compound Concentration %	Zone of Inhibition, mm
3.0	13
1.0	10
0.3	8
Control	0

Candida albicans: Test conditions similar to those for Sporotrichum schenckii, above.

Test Compound Concentration %	Growth
0.18	?
0.06	0
0.018	+4
Control	+5

[221]

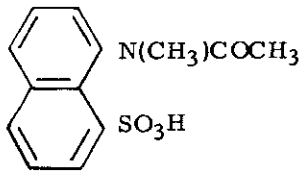
USE Medicinal.

111. 1-NAPHTHALENESULFONIC ACID, 8-N-METHYLACETAMIDO-

ALTERNATIVE NAME N-Acetyl-N-methyl-8-amino-1-naphthalenesulfonic acid.

MOLECULAR FORMULA $C_{13}H_{13}NO_4S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 279.308.

TESTS In vitro. 10-fold dilutions of test compound added to spore suspension in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 1000 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm. [55]

TOXICITY Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight; exposure 24 hours. No injury. [297]

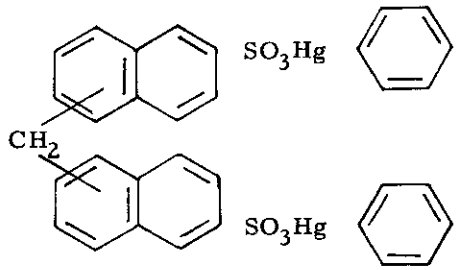
USE Protectant of materiel.

112. 2-NAPHTHALENESULFONIC ACID, x,x'-METHYLENEDI-, BIS(PHENYLMERCURY) SALT

ALTERNATIVE NAME Phenylmercuric dinaphthylmethane disulfonate.

MOLECULAR FORMULA $C_{33}H_{24}Hg_2O_6S_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White, amorphous solid. Molecular weight, 981.874. Almost insoluble in water [104].

112. 2-NAPHTHALENESULFONIC ACID, x,x'-METHYLENEDI-, BIS(PHENYLMERCURY) SALT (Concluded)

TESTS In vitro. Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, and Microsporum sp: Glucose medium, containing peptone. Test compound added and incubated for 21 days at 25°C; MED, 0.0041%. [104]

Candida albicans Martin and Jones, et al, and Monilia albicans Zopf.: Lemco medium, half strength beerwort instead of water; MED, 0.006%. Aspergillus niger (Van Tiegham), and Penicillium citrinum: Czapek's medium, plus 0.1% asparagine; MED, 0.011%. Rhizopus nigricans (Ehrenberg): Czapek's medium, plus 0.1% asparagine; MED, 0.01%. Penicillium notatum: Czapek's medium, plus 0.1% asparagine; MED, 0.006% [104].

TOXICITY Mice: LD_{50}, 70 mg/kg, p.o.; 25 mg/kg, i.p. Death occurred in 14 days. [104]

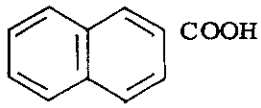
USE Protectant of materiel; medicinal.

113. 2-NAPHTHOIC ACID

ALTERNATIVE NAMES β-Naphthalenecarboxylic acid; β-Naphthoic acid.

MOLECULAR FORMULA $C_{11}H_8O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [118], white [100], monoclinic needles [118]. Molecular weight, 172.174. Melting point, 164-165°C [228], 184-185°C [192], 185°C [118]. Boiling point, 300°C. Specific gravity, 1.077 (100/4°C). Very soluble in alcohol, ether. Soluble in sodium hydroxide solution. [118] Stable [100].

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading at 96 hours. 250 ppm inhibited growth 100%. [100]

TOXICITY Animals. Hyperpnea, prostration [261].

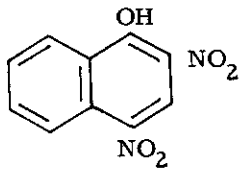
USE Protectant of materiel.

114. 1-NAPHTHOL, 2,4-DINITRO-

ALTERNATIVE NAME 2,4-Dinitro-α-naphthol.

MOLECULAR FORMULA $C_{10}H_6N_2O_5$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow needles [118]. Molecular weight, 234.164. Melting point, 138°C [118], 164°C [250]. Soluble in acetic acid. Slightly soluble in alcohol. Very slightly soluble in hot water. [118]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

ppm	% Inhibition
10	86
20	86
30	88
40	90
60	92
250	100

[52]

A. niger (Van Tiegham):

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	8.4

x 10^{-5} M	10	7.5	5.0	2.5	1.0
% inhibition	85	85	78	70	58
	82	79	77	66	56

[228]

114. 1-NAPHTHOL, 2,4-DINITRO- (Concluded)

TOXICITY

Animal	Dose	mg/kg	Route	Time of Death
Dog	LD	30-60	i.v.	30 min
Guinea pig	LD	80-100	s.c.	15-30 min
Frog	LD	60	s.c.	30 min
Pigeon	LD_{50}	18.5	i.m.	
Pigeon	LD	15	i.p.	

[120]

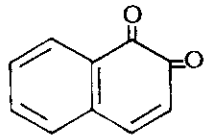
USE Protectant of materiel.

115. 1,2-NAPHTHOQUINONE

ALTERNATIVE NAMES β-Naphthoquinone; 1,2-Dihydro-1,2-diketonaphthalene.

MOLECULAR FORMULA $C_{10}H_6O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow-red needles. Molecular weight, 158.148. Decomposes, 115-120°C. [118] Soluble in water, alcohol, ether, benzene [118]; concentrated sulfuric acid [228].

TESTS In vitro. Aspergillus niger (Van Tiegham): Growth of inoculum (nutrient agar inoculated with 1 drop of spore suspension and incubated 96 hours at 30°C) inhibited 71% by 250 ppm of test compound (5 ml in 95 ml distilled water, plus wetting agent).

Stemphylium sarcinaeforme Cav.: Spore germination test on depression slide (0.4 cc of 14 day-old cultured spore suspension, 0.2 cc of test compound per slide, depositing compound at bottom of cavity; dried, and cultured 17 hours). MED, 1 μg/sq cm. [55]

Alternaria oleraceae Milb., and Sclerotinia fructicola (Wint.) Rehm.: Glass slide spore germination test, as recommended by the Council of the American Phytopathological Society. ED_{50}, 0.01-1 ppm. [189]

In vivo. Alternaria solani (Ell. and Mart.) J. and G., and Sclerotinia fructicola (Wint.) Rehm.: Spray test on tomato foliage. ED_{95}, 800 ppm. [189]

115. 1,2-NAPHTHOQUINONE (Concluded)

TOXICITY Animals. Albino and hooded rats, weighing 130-200 g: MLD, 250 mg/kg, s.t. [38].

Fish screening test, USDI. 8 fish, 4 inches or less, each species; test compound concentration, 5 ppm by weight. Salmo trutta (brown trout), death in 1 hour. Lepomis macrochirus (bluegill sunfish), and Carassius auratus (goldfish): Death in 1.5 hours. [297]

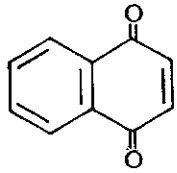
USE Protectant of materiel; medicinal; agricultural.

116. 1,4-NAPHTHOQUINONE

ALTERNATIVE NAMES 1,4-Dihydro-1,4-diketonaphthalene; α-Naphthoquinone.

MOLECULAR FORMULA $C_{10}H_6O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals. Molecular weight, 158.148. Melting point, 124-125°C [228]. Sublimes at 100°C. Very soluble in hot alcohol, carbon disulfide, glacial acetic acid, benzene, chloroform. Soluble in ether. Very slightly soluble in cold water. [118]

TESTS In vitro. Alternaria oleracea Milb., and Sclerotinia fructicola (Wint.) Rehm.: 0.1-1 ppm inhibited spore germination 50% [189].

Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 100% [228].

In vivo. Alternaria solani (Ell. and Mart.) J. and G.: 1000 ppm spray controlled foliage infection in tomato plants (ED_{95}) [189].

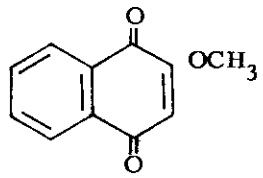
TOXICITY Mice: 7.8 mg/kg, i.p., daily for 5 days, lethal. MTD, 3.9 mg/kg, i.p. [260]. Rats (albino or hooded): 100 mg/kg, s.t., lethal [281].

USE Protectant of materiel; agricultural.

117. 1,4-NAPHTHOQUINONE, 2-METHOXY-

MOLECULAR FORMULA $C_{11}H_8O_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light yellow, feathery crystals [231]. Molecular weight, 188.174. Melting point, 184.8-185°C. Soluble in boiling alcohol. Insoluble in water. Unstable to alkalies. [231]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	Trace

x 10^{-5} M	10	7.5	5.0	2.5	1.0
% inhibition	100	Trace	82	35	13

250 ppm inhibited growth 100%. [231]

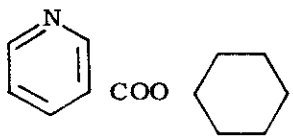
10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 1000 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [231]

USE Protectant of materiel.

118. NICOTINIC ACID, CYCLOHEXYL ESTER

MOLECULAR FORMULA $C_{12}H_{15}NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Liquid [81]. Molecular weight, 205.248. Boiling point, 144.5°C (4.1 mm Hg). Specific gravity, 1.0941 (25/4°C). Refractive index, 1.5177 (25°C). Soluble in alcohol. [81]

118. NICOTINIC ACID, CYCLOHEXYL ESTER (Concluded)

TESTS In vitro. Trichophyton (gypseum) mentagrophytes: Melted agar, seeded with conidia; undiluted test compound placed in 3-5 mm area on plate; incubated at 30°C. 1.5 cm inhibition area at 1 and 2 weeks. [210]

10-fold dilutions of test compound added to spore suspension in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 10,000 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 1000 ppm. [55]

Aspergillus niger (Van Tiegham): 1 drop of spore suspension and various concentrations of test compound in nutrient toxic agar; incubated 96 hours at 30°C.

ppm	% Inhibition
250	100
10	94
7.5	52
5	24
2.5	15
1	12

[229]

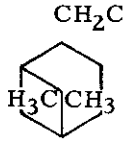
USE Protectant of materiel.

119. 2-NORPINANEACETIC ACID, 6,6-DIMETHYL-

ALTERNATIVE NAME Hydronopic acid.

MOLECULAR FORMULA $C_{11}H_{18}O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Solid. Molecular weight, 182.254. Melting point, 56-58°C. Easily soluble in organic solvents. Insoluble in water. Stable. [102]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound, inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	Trace	63	45	28

250 ppm inhibited growth 100%. [231]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [102]

USE Protectant of materiel.

120. NYSTATIN

ALTERNATIVE NAME Fungicidin.

SOURCE Streptomyces noursei.

MOLECULAR FORMULA $C_{46}H_{77}NO_{19}$ or $C_{46}H_{83}NO_{18}$ (proposed)

PHYSICAL AND CHEMICAL PROPERTIES Yellow powder [120]. Gradual decomposition above 160°C, without melting at 250°C. Slightly soluble in methanol, ethanol, butanol, dioxane. Insoluble in water, pyridine, dimethyl formamide, glacial acetic acid, 0.05 N methanolic HCl, sodium hydroxide. No loss in cold; unstable at pH 2 or 9. [121]

TESTS In vitro. Coccidioides immitis: Saline solution (pH 7.4) added to asparagine media in test tubes (0.1-1000 μg/ml of medium). 1 drop of saline suspension of C. immitis added to each tube; incubated at 35°C. 100 μg/ml suppressed growth during 30-day observation period. Smaller amounts of compound prevented growth for a few days, but with continued incubation growth occurred. [107]

Histoplasma capsulatum: 14 strains tested in mycelial phase, grown on Sabouraud's glucose agar at room temperature. All were inhibited with as little as 2.5 units[1] in first 3-5 days, while most controls developed quite visible colonies. At 7 days, 13 of the 14 strains showed inhibition with 5 units, and only one strain was growing. At 10 days, 7 strains showed inhibition with 10 units, and at 25 days, 6 showed inhibition with 20 units. At this time only 3 strains were growing in the presence of 50 units/ml, but the size of the colonies was markedly smaller than in the controls. [74]

H. capsulatum: 8 strains in yeast phase, grown on cysteine blood agar at 37°C. Inhibition obtained with 10 units in 1 strain for 3 days, in 2 strains for 10 days. 20 units inhibited 6 strains for about 10 days, and 50 units inhibited all strains except 1 which was also considerably resistant in mycelial phase. [74]

Concentrations of 1.25-6.25 μg/ml inhibited Blastomyces brasiliensis, B. dermatitidis, Coccidioides immitis, Cryptococcus neoformans, Epidermophyton floccosum, Histoplasma capsulatum, Microsporum audouini, M. canis, Trichophyton mentagrophytes, T. rosaceum, T. rubrum. Strains of Candida albicans and Geotrichum spp inhibited by

/1/ 2500 units equivalent to 1 mg.

1.25-12.5 μg/ml. Concentrations of 575 units/ml (230 μg/ml) inhibited Entamoeba histolytica [121].

In vivo. Rabbits: Infected i.v. with Candida albicans. Mortality reduced 62% by 40 mg, s.c., daily for 5 days. No effect from oral administration due to poor absorption. [74]

Mice, white: Inoculated i.p. with 0.5 ml of saline spore suspension of Coccidioides immitis (100-700 spores). Infected mice divided into 3 groups: 50 used as controls and given physiologic saline; 2 groups of 100 each treated s.c., one group receiving 0.5 mg, the other 1.0 mg, daily for 5 days, rest 2 days, for 30 days. Controls began dying on 10th day, with 92% dead by 18th day. 75 days after infection, or 45 days after treatment was discontinued, the 0.5 mg group had had 28% mortality, the 1.0 mg group 13%. [107]

S.c. doses of 25-150 mg/kg protected mice against infections with Candida albicans, Histoplasma capsulatum, Coccidioides immitis, Cryptococcus neoformans, Sporotrichum schenckii. In mice infected i.v. with Candida albicans, there was a high protection rate following oral doses of 4 mg. In rabbits infected with C. albicans, doses of 40 mg/kg, s.c. or i.v., reduced mortality from 100% to 62%. Median protective dose against Blastomyces dermatitidis in mice was 0.8 mg/kg, i.p., daily for 10 days. [121]

TOXICITY Man. Little or no toxic action; tolerated in infants, even those in very poor condition. [74] Daily oral doses up to 1.25 g for 30 days well tolerated; no significant side effects. [121] I.m. and i.v. injections followed by chills, fever, malaise [209].

Animals. Mice tolerated repeated daily i.p. doses of 24 mg/kg, or 50 mg/kg, s.c., for 10 days. Repeated oral administration of 300 mg/kg in rats and 1000 mg/kg in dogs non-toxic. 0.5 mg, s.c., daily for 58 days well tolerated in hamsters; single doses of 80 mg/kg toxic. [121] Repeated subcutaneous injections in mice were accompanied by necrosis, but no gross accumulation of toxic effects noted following a total of 1250 mg/kg during 8-day period [30].

USE Medicinal: intermediate and deep mycoses [21, 127, 252].

121. PARIS GREEN

ALTERNATIVE NAMES Schweinfurtergrün; Emerald green; French green; Mitis green; Copper acetoarsenite; Cupric acetoarsenite.

MOLECULAR FORMULA $(CuO)_3As_2O_3 \cdot Cu(C_2H_3O_2)_2$

121. PARIS GREEN (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Emerald-green powder. Molecular weight, 1013.708. Soluble in dilute acids. Insoluble in water. [53]

TOXICITY Man. Highly toxic. Probable LD, 5-50 mg/kg. [101] Causes troublesome skin lesions, resulting at an early stage in an edematous condition, with inflammation and finally ulceration [250].

Animals.

Animal	Dose	mg/kg	Route
Guinea pig	LD	30	p.o.
Rat	MLD	300	p.o.
Rat	LD	22[1]	p.o.
Frog	MLD	10	s.c.

[120]

USE Protectant of materiel: wood preservative [101]. Agricultural.

CAUTION Handlers should use protective equipment [250].

122. 2,4-PENTANEDIONE

ALTERNATIVE NAMES Pentanedione-2,4; Diacetylmethane; Acetoacetone.

MOLECULAR FORMULA $C_5H_8O_2$

PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid. Solidifies when cooled to lustrous, pearly spangles. Unpleasant odor. [53] Molecular weight, 100.114. Melting point, -23.5°C. Boiling point, 139°C (746 mm Hg). [118] Specific gravity, 0.9753 (20/20°C). Soluble in water (acidified by hydrochloric acid), alcohol, chloroform, ether, benzene, acetone, glacial acetic acid. [53]

/1/ Approximately.

122. 2,4-PENTANEDIONE (Concluded)

TESTS In vitro.

	µg/sq cm	% Inhibition
Sclerotinia fructicola (Wint.) Rehm.	1000	100
	100	100
	10	100
	1	100
Stemphylium sarcinaeforme Cav.	1000	100
	100	60
	10	0

[53]

TOXICITY LD_{50} in rats, 1000 mg/kg, p.o. [47]

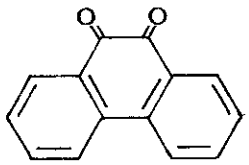
USE Agricultural.

CAUTION Fire hazard [250].

123. PHENANTHRENEQUINONE

MOLECULAR FORMULA $C_{14}H_8O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow or yellow-orange, needle-like powder. Molecular weight, 208.204. Melting point, 207°C. Boiling point, 360°C. [118] Sublimes above 360°C [295]. Specific gravity, 1.4045 [53], 1.405 [118]. Soluble in sulfuric acid, benzene, glacial acetic acid, hot alcohol [53]. Very slightly soluble in water, ether [118]. Stable.

TESTS In vitro. Aspergillus niger: 250 ppm inhibited growth 74% [229].

Alternaria oleracea Milb., and Sclerotinia fructicola (Wint.) Rehm.: ED_{50}, 0.01-0.1 ppm [189].

In vivo. Alternaria solani (Ell. and Mart.) J. and G.: 400 ppm controlled infection on tomato plant foliage [181].

123. PHENANTHRENEQUINONE (Concluded)

Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 oranges, ethylene gas treated to accelerate rot, dipped, dried, and stored at 70°F for 3 weeks. Treatment with compound did not prevent rot. [295]

TOXICITY LD in mice, 165 mg/kg, i.p. [47]

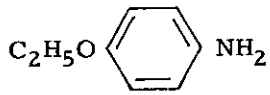
USE Agricultural: control of foliage diseases.

124. p-PHENETIDINE

ALTERNATIVE NAME p-Ethoxyaniline.

MOLECULAR FORMULA $C_8H_{11}NO$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Clear, oily liquid [69]. Molecular weight, 137.176. Freezing point, 2.4°C [118], 3.0°C [69], 4.65°C [72]. Boiling point, 249.6°C [69], 254.2°C [118], 248.59°C [72], 254.7°C [228]. Specific gravity, 1.0613 (15/4°C) [118], 1.061 (25/25°C) [69]. Refractive index, 1.56101. Vapor pressure, 0.0092 mm Hg (25°C) [72]. Soluble in alcohol, ether, carbon tetrachloride. Slightly soluble in water. [69]

TESTS In vitro. Aspergillus niger (Van Tiegham): 250 ppm inhibited growth 25% [228].

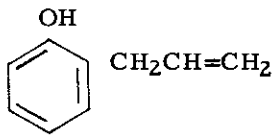
TOXICITY Animals. Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), Carassius auratus (goldfish): 2 fish each species; concentration level, 5 ppm by weight; exposure 24 hours. No injury. [297]

USE Protectant of materiel.

125. PHENOL, o-ALLYL-

MOLECULAR FORMULA $C_9H_{10}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 134.170. Boiling point, 99-101°C (13 mm Hg). Soluble in alkalies, organic solvents. [118]

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 250 ppm inhibited growth 100%. [235]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm.

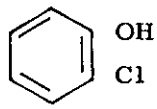
USE Protectant of materiel.

126. PHENOL, o-CHLORO-

ALTERNATIVE NAMES o-Chlorophenol; 1-Chloro-2-hydroxybenzene.

MOLECULAR FORMULA C_6H_5ClO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [118]. Unpleasant, penetrating odor [53]. Molecular weight, 128.557. Boiling point, 174.9°C [72]. Vapor pressure, 1.5573 mm Hg (25°C). Specific gravity, 1.26346 [72], 1.241 (18/15°C) [118]. Refractive index, 1.55939 [72], 1.5473 (40°C) [118]. Soluble in alcohol, ether [118]. Slightly soluble in water [53].

TESTS In vitro. Rhizopus nigricans: 0.05% of test compound inhibited growth [114].

Aspergillus niger (Van Tiegham): Test compound in nutrient medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7); incubated 48 hours at 37°C. 0.03% inhibited growth. [181]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard: 2,500,000 conidia per plate; Sabouraud's dextrose agar, plus 10% horse serum; 1 ml of 0.1% alcohol solution of test compound; incubated 5 days at 28-30°C. Decreased infestation. Agar disks from 15-day culture in 1% solution of test compound for 1 minute, rinsed, subcultured on Sabouraud's medium for 21 days. Did not abolish growth. [312]

Spores of Stemphylium sarcinaeforme, and Monilinia fructicola: LD_{50}, >1000 μg/sq cm [138].

Aspergillus niger:

x 10^{-4} M	25	12.5	10	7.5	5.0	2.5	1.0
% inhibition	76	40	42	26	19	1	3
			47	40	30	19	11
			31				4

[228]

TOXICITY Man. Highly toxic. Rapidly absorbed through skin; causes severe burns; slight liver and kidney damage; apparent narcotic effect; respiratory depression. [71] Severe irritation to conjunctiva [250].

Animals.

Animal	LD, mg/kg	Route
Rabbit	120	i.v.
Rat	670[1]	p.o.
Rat	950[1]	s.c.
Frog	400	s.c.

[120]

USE Protectant of materiel: paper [111]. Agricultural.

CAUTION Handlers should wear protective clothing and chemical safety goggles [250].

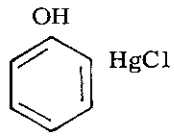
/1/ 50% solution in olive oil.

127. PHENOL, o-(CHLOROMERCURI)-

ALTERNATIVE NAMES o-Hydroxyphenylmercuric chloride; o-Chloromercuriphenol.

MOLECULAR FORMULA C_6H_5ClHgO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White to faint pink crystals [53, 95]. Molecular weight, 329.167. Melting point, 143-145°C [53]; 147-152°C [192]. Soluble in hot water, alkalies, alcohol [53]; sodium hydroxide solutions [192].

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: 1 μg/sq cm stopped spore germination [55].

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, and Epidermophyton floccosum (Harz) Langeron and Milochevitch: Sabouraud's agar, streaked with 10-day agar slant culture of test organism. Growth inhibited completely by 25 ppm threshold concentration. Both fungicidal and fungistatic. [195]

TOXICITY Man. Probable LD, 5-50 mg/kg [101]. Dust or strong solution causes blistering of skin unless exposed parts are promptly washed [53].

Animals.

Animal	Dose	mg/kg	Route	Reference
Mouse	LD_{50}	36	s.c.	
Mouse	LD_{50}	23	i.v.	
Rat	MLD	100	s.t.	61, 297
Rat	MLD	25[1]	i.p.	61, 297
Rat[2]	MLD	100	s.t.	148

COMPARATIVE TOXICOLOGY Less corrosive than mercuric chloride, but systemic toxicity is probably almost as great [101.

USE Medicinal; agricultural.

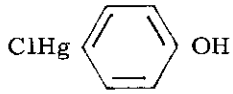
/1/ Reference 61: daily for 1 week. /2/ Albino or hooded.

128. PHENOL, p-(CHLOROMERCURI)-

ALTERNATIVE NAME p-Chloromercuriphenol.

MOLECULAR FORMULA C_6H_5ClHgO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 329.167. Melting point, 224-225°C.

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: MED, 1 μg/sq cm. Stemphylium sarcinaeforme Cav.: MED, 10 μg/sq cm. [55]

TOXICITY Rats: MLD, >500 mg/kg, s.t.; 50 mg/kg, i.p. [61,297]

PHYTOTOXICITY Corn seed, var. Silver King (Wisconsin No. 7): Inhibition of primary root by test compound in aqueous solution upon germination of seed at 27°C. Triplicate tests. Results after 4 days expressed as percentage of growth inhibited compared to that resulting from a 2,4-D standard solution arbitrarily designated as 100%. 28% decrease with test compound. [277]

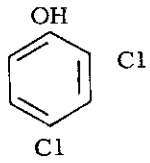
USE Medicinal.

129. PHENOL, 2,4-DICHLORO-

ALTERNATIVE NAME 2,4-Dichlorophenol.

MOLECULAR FORMULA $C_6H_4Cl_2O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless needles [118]; white, low-melting solid [53]. Molecular weight, 162.006. Melting point, 45°C. Boiling point, 210°C. Soluble in alcohol, carbon tetrachloride. Slightly soluble in water.

129. PHENOL, 2,4-DICHLORO- (Concluded)

TESTS *In vitro*. *Chaetomium globosum*, and *Aspergillus niger* (Van Tiegham): 1% of test compound and undiluted streak incubated in nutrient agar for 72 hours at 30°C. Prevented infestation. [70]

A. niger (Van Tiegham): 1.9% of compound (dry cloth weight basis), incubated 1-3 weeks at 30°C. Impregnated cloth resisted growth of organism. [70]

A. niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	100	83	36
	100	100	100	54	27
	100	Trace	Trace	82	33

x 10^{-5} M	7.5	5.0	2.5	1.0
% inhibition	22	15	10	11
	31	25	24	18

250 ppm inhibited growth 100%. [228]

In vivo. *Rhizopus nigricans* (Ehrenberg): 0.01% of test compound active against infection in pea and peanut seeds [114].

TOXICITY Man. Extremely irritating to skin and mucous membranes [228].

Animals. Rats: LD_{50}, 580 mg/kg, p.o. (20% solution in fuel oil); LD, 1730 mg/kg, s.c. [120]

USE Protectant of materiel; medicinal; agricultural.

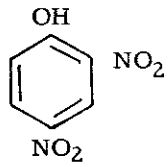
CAUTION Handlers should wear protective clothing and equipment [228].

130. PHENOL, 2,4-DINITRO-

ALTERNATIVE NAME DNP.

MOLECULAR FORMULA $C_6H_4N_2O_5$

STRUCTURAL FORMULA



130. PHENOL, 2,4-DINITRO- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Yellow, orthorhombic crystals [118]. Molecular weight, 184.108. Melting point, 114-115°C [53]. Soluble in ether, benzene, chloroform. Slightly soluble in water [53].

TESTS In vitro. Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	100	83	43
	100	100	Trace	75	71

x 10^{-5} M	50.0	10.0	7.5	5.0	2.5	1.0	0.5	0.1
% inhibition	100	74		57		23	7	2
		79	78	70	54	33		
		76	74	65	51	31		
		80	79	68	53	28		

250 ppm inhibited growth 100%. [228]

TOXICITY Man. Marked fatigue, tremendous thirst, profuse sweating, flushing of face; nausea, vomiting, abdominal pain, occasionally diarrhea; restlessness, anxiety, excitement occasionally followed by convulsions; rise in body temperature which is roughly proportional to the toxic dose, often leading to severe hyperpyrexia; tachycardia, hyperpnea, dyspnea, cyanosis and sometimes muscle cramps; loss of consciousness, death. [101]

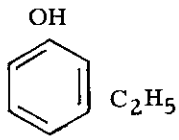
USE Protectant of materiel: wood, rubber [99].

CAUTION Dangerous fire hazard when dry.

131. PHENOL, m-ETHYL-

MOLECULAR FORMULA $C_8H_{10}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid [53]. Molecular weight, 122.160. Melting point, -4°C [53,118]. Boiling point, 214°C. Specific gravity, 1.001. Very slightly soluble in water. Miscible with alcohol and ether. [53]

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: 1000 μg/sq cm completely stopped spore germination. Stemphylium sarcinaeforme Cav.: 1000 μg/sq cm did not inhibit spore germination. [53]

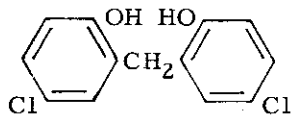
USE Agricultural.

132. PHENOL, 2,2'-METHYLENEBIS(4-CHLORO-

ALTERNATIVE NAMES Dichlorophene; Bis(5-chloro-2-hydroxyphenyl) methane; 2,2'-Dihydroxy-5,5'-dichlorodiphenyl methane; G-4; 2,2'-Methylenebis(4-chlorophenol); o,o'-Methylenedi-(p-chlorophenol).

MOLECULAR FORMULA $C_{13}H_{10}Cl_2O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light tan, free-flowing powder. Weakly phenolic odor. [53] Molecular weight, 269.124. Melting point, 164°C (min.). Vapor pressure, 10^{-4} mm Hg (100°C), 10^{-10} mm Hg (25°C) (calc.). [53] Soluble (g/100 ml solvent at 25°C) in water, 0.003; acetone, 80.0; benzene, 1.4; butanol, 42.3; tert.-butanol, 54.6; "Carbitol," 1.4; carbon tetrachloride, 0.1265; ethyl acetate, 1.0; ethyl alcohol, 53.0; ethylene dichloride, 2.68; isopropyl alcohol, 54.0; methylethyl ketone, 75.0; mineral spirits, 0.055; petroleum ether, 0.0084; propylene glycol, 45.0; Stoddard's solvent, 0.2; toluene, 1.6. [246]

TESTS In vitro. Aspergillus niger (Van Tiegham): Test compound added to salt medium plus dextrose. Mycelia weighed after 20 days.

Compound Concentration ppm	Mycelia Weight	Growth Decrease, %
0	150	
10	125	17
20	60	60
30	15	90

[313]

A. niger (Van Tiegham): Test compound added to medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7). 0.0063% inhibited growth. [181]

1 ml of a 1% alcohol solution of test compound, added to Sabouraud's agar plus 10% horse serum, decreased infestation:

	Decreased Infestation Zone, mm
Candida albicans, Martin and Jones, et al	7-4
Trichophyton (gypseum) mentagrophytes	15-4.5
Debaryomyces neoformans	10.5-3

[94]

Stemphylium sarcinaeforme spores: LD_{50}, 58.9 μg/sq cm. Monilinia fructicola spores: LD_{50}, 0.3 μg/sq cm. [138]

	Minimum Inhibiting Concentration, %
Chaetomium globosum	0.3 (on cellulose)
Aspergillus niger (Van Tiegham)	0.3 (on cellulose)
A. niger (Van Tiegham)	1.75 (on wool)

[138]

A. niger:

x 10^{-4} M	5.0	2.5	1.0	0.75	0.5	0.25	0.1	0.05	0.01
% inhibition	100	89	72	65	57				
	100	81	65	58	53				
	100		66		57	42		18	
	100	75	71		55	44	26	23	6
	Trace		62		60		31	28	9

[228]

In vivo. Venturia inaequalis: Compound not effective in protecting apple foliage against infection. [138]

TOXICITY Man. Probable LD, 500-5000 mg/kg. 1% not irritating to skin. [101]

Animals. 0.1% fed to rats in diet for 2 weeks had no adverse effects.

Animal	Dose	mg/kg	Route	Reference
Dog	LD_{50}	3000[1]	p.o.	70
Guinea pig	LD_{50}	1250	p.o.	70, 180
Mouse	LD	500	i.p.	260
Mouse	LD	250	i.p.	260
Rat, white	LD_{50}	2000[1]	p.o.	70

COMPARATIVE TOXICOLOGY Compound shows promise as being one of the best of the phenolic derivatives for use on fabrics; up to 2% concentration apparently lacks the skin irritating characteristics of other phenolic compounds. [22]

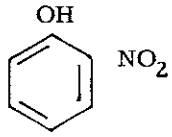
USE Protectant of materiel: mildew-proofing agent for cotton yarn, thread, fabrics [22, 168]; preservative for liquid and paste products, glues, adhesives [53]; leather [14]. Medicinal. Agricultural.

/1/ Approximately.

133. PHENOL, o-NITRO-

MOLECULAR FORMULA $C_6H_5NO_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light yellow, monoclinic needles or prisms [118]. Aromatic odor [192]. Molecular weight, 139.108. Melting point, 44.25-44.9°C [228], 45°C [118]. Boiling point, 214.5°C. Specific gravity, 1.657 (20°C) [118]; 1.2942 (40°C) [228]. Freely soluble in hot water, alcohol, benzene, ether, carbon disulfide, alkaline hydroxides [118, 192].

TESTS In vitro. Compound incorporated in nutrient agar. Plates inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); incubated for 48 hours at 30°C, at 85% relative humidity. Radii of the colonies measured at 24-hour intervals until growth in the normal control plate reached periphery of plate.

	% Inhibition		
	Aspergillus niger	Penicillium citrinum	Trichoderma sp
1×10^{-3} M	100	100	100
1×10^{-4} M	24	16	47
5×10^{-5} M	14	8	32
1×10^{-5} M	9	0	7
5×10^{-6} M	6	0	2

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Spore germination: Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 10,000 ppm. [123]

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	100	86	55
	100	100	Trace	70	39
	100	100	Trace	71	42
	100	100	95	71	37

x 10^{-5} M	10	7.5	5.0	2.5	1.0
% inhibition	60	52	30[1]	21	8[1]

LD_{50}, 25 ppm. [228]

/1/ Average.

133. PHENOL, o-NITRO- (Concluded)

TOXICITY Animals.

Animal	Dose	mg/kg	Route
Cat	LD	600	s.c.
Dog	LD	100	i.v.
Mouse	LD	600	i.m.
Rabbit	LD	1700	s.c.
Frog	LD	300	s.c.

[120]

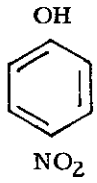
USE Protectant of materiel.

134. PHENOL, p-NITRO-

ALTERNATIVE NAME p-Nitrophenol.

MOLECULAR FORMULA $C_6H_5NO_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellowish, monoclinic, prismatic crystals [53]. Molecular weight, 139.108. Melting point, 111.4-114°C (sublimes). Decomposes, 273°C. Specific gravity, 1.479-1.495 (20°C). [53] Vapor pressure, 0.0828 mm Hg (100°C). Soluble in hot water, alcohol, ether. [53]

TESTS In vitro. Stemphylium sarcinaeforme spores: LD_{50}, approximately 25 μg/sq cm. Monilinia fructicola spores: LD_{50}, approximately 50 μg/sq cm. [138]

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0	0.5	0.1
% inhibition	100	66	54	30	26		
	99	69	57	35	17	4	-5
	83	60	47	26	7		

x 10^{-4} M	9.7	7.3	4.85	2.42	0.97	0.49	0.097
% inhibition	76	63	49	28	16	12	9
	77	60	48	29	20	7	8

x 10^{-5} M	10	7.5	5.0	2.5	1.0
% inhibition	14	9	2	-1	2

TOXICITY Man. In concentration of 0.75%, p-nitrophenol has no adverse effect on the skin [175]. Patch tests reveal no irritation [112]. Tests have failed to produce any skin irritation or other toxic symptoms from application of p-nitrophenol in concentration higher than those advocated for mould inhibition, even in oily solutions [244].

Animals. LD in dogs, 0.01 g/kg, i.v. [303]. No irritation noted in dogs and horses when leather preserved with p-nitrophenol was placed on skin of these animals, although the protective levels of 0.25-0.50% was exceeded 3- to 4-fold.

COMPARATIVE TOXICOLOGY Concentrations at which various materials exhibit fungistatic and fungicidal power against Aspergillus niger growing in modified Czapek's broth for 28 days at 25°C:

Compound	Lowest Concentration to Inhibit Growth	pH Change[1]	Lowest Concentration to Kill Spores	pH Change[1]
Phenol	1:1400-1:1600	0	1:1400-1:1600	0
Resorcinol	1:50-1:100	0	1:50-1:100	0
o-Cresol	1:2000-1:3000	0	1:2000-1:3000	0
m-Cresol	1:2000-1:3000	0	1:2000-1:3000	0
Sodium salt	1:12,500-1:15,000	+0.3	1:4000-1:5000	+0.6
o-Nitrophenol	1:20,000-1:30,000	0	1:2000-1:3000	-0.2
m-Nitrophenol	1:2500-1:5000	+0.1	1:2500-1:5000	+0.1
p-Nitrophenol	1:7000-1:8000	-0.2	1:7000-1:8000	-0.2
p-Chlorophenol	1:8000-1:9000	0	1:4000-1:5000	0
Sodium salt	1:12,500-1:15,000	+0.3	1:4000-1:5000	+0.6

[24]

USE Protectant of materiel: leather (p-nitrophenol best of all substances tested, a very high degree of resistance being conferred by addition of 0.3% of compound calculated on the weight of the leather [262]) [22, 111]; paper, rubber, textiles [111]. Medicinal: ringworm in calves, horses, rabbits; "athlete's foot." [244]

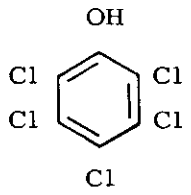
135. PHENOL, PENTACHLORO-

ALTERNATIVE NAME Pentachlorophenol.

MOLECULAR FORMULA C_6HCl_5O

/1/ Of control broth, caused by addition of test compound.

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White powder or needle-like crystals (pure), dark-colored flakes (technical) [318]; monoclinic prisms [117]. Chlorophenolic odor. Molecular weight, 266.353. Melting point, 190°C [53], 150-178°C [228], 191°C (pure) [118]. Boiling point, 310°C (pure); decomposes, >293°C. [53,118] Specific gravity, 1.978 (22/4°C) [53,118]. Vapor pressure, 0.12 mm Hg (100°C); volatile in steam. [180] Soluble (g/100 g solvent at 25°C) in acetone, 53; benzene, 11; butyl "Carbitol," 156; butyl "Cellosolve," 150; carbon tetrachloride, 4; castor oil, 17; coal tar creosote (AWDA 1), 54; coconut oil, 40; cottonseed oil, 35; deobase oil, 4; diacetone alcohol, 193; dibutyl phthalate, 70; o-dichlorobenzene, 12; diglycol, 100; ether, 148; ethyl alcohol (formula 30), 143; fuel oil, 12; linseed oil, 26; menhaden oil, 36; methanol, 57; mineral oil, light, 2; neat's-foot oil, 22; olive oil, 19; perilla oil, 38; petrolatum, white, 2; pine oil, 89; soybean oil, 35; sperm oil, 20; stinesol, 3; Stoddard's solvent (40°C), 4; tetrachloroethane, 8; toluene, 14; turkey red oil, 8; oil of turpentine, 10; water, 0.0016; xylene, 16. [318] Soluble in dilute alkalies, "Carbitol," "Cellosolve." [53]

TESTS In vitro.

	Concentration % for Inhibition	% for Kill
Rhizopus nigricans	0.05	0.05
Rhizoctonia solani	0.002	0.002
Chaetomium globosum	0.0035	0.0035
Hormiscus gelatinosum	0.01	0.02
Polyporus tulipiferous	0.002	0.0035
Aspergillus flavus	0.005	0.01
Lenzites trabea	0.002	0.002
Ceratostomella pilifera	0.0035	0.0035
Trichophyton interdigitale	0.001	0.001
T. rosaceum	0.005	0.1
Poria luteofibrata		0.0025

	Concentration in Agar % for Inhibition
Pullularia sp	0.0016
Myrothecium verrucaria (Metarrhizium glutinosum)	0.0016
Chaetomium globosum	<0.00039
Oothecium sp	<0.00039
Aspergillus ustus	0.0016
A. niger	0.00078

[314]

	Concentration on Fabric[1] % for Inhibition
Chaetomium globosum	0.06
Stemphylium sp	0.12-0.16
Hormodendrum sp	0.98

[314]

Stemphylium sarcinaeforme spores: LD_{50}, approximately 2.5 μg/sq cm. Monilinia fructicola spores: LD_{50}, approximately <1.0 μg/sq cm. [138]

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.2	1.0	0.9	0.7
% inhibition	100	100	100	100	100	86	93	Trace

x 10^{-5} M	10	7.5	6.0	5.0	4.0	3.0	2.5	2.0	1.2	1.0	0.5	0.1
% inhibition			78			66			51			
			83	70	64	57		54		45	34	18
				77			62			50	42	20
				88			64			57	45	27
	77	65		58			46			33		

250 ppm inhibited growth 100%. [228]

TOXICITY Man. Dust and vapor irritating to mucous membranes; may provoke violent sneezing. Solid, and water solutions stronger than 1%, irritating to skin. [95, 96, 180] Skin absorption [325]. In commercial production and use of pentachlorophenol, no cases of acute intoxication reported in handlers [155].

Animals. Moderate chronic toxicity; compound rapidly eliminated from the body. Dust irritating to nose and throat. Marked irritation and damage to eyes of guinea pigs, rabbits, and rats, depending on concentration. [325] 2% pentachlorophenol applied to skin of rats produced severe irritation; 10% produced death. [174] No fatalities in rats and dogs fed 3.9-10 mg in diet for 10-28 days [180].

Animal	Dose	mg/kg	Route	Time of Death	Reference
Dog	MLD	135	s.c.		120
Mouse	MLD	56	s.c.		120
Rat	LD_{50}	78[2]	p.o.		120
Rat	LD_{50}	125-200	p.o.		120
Rat	LD_{50}	210	p.o.		47, 95
Rat	LD_{50}	125-200	s.t.		47
Rabbit	MLD	550	p.o.		120
Rabbit	MLD	257	p.o.		120
Rabbit	MLD	512.5	s.c.		120
Rabbit	MLD	135.5	i.p.		120
Rabbit	LD	7090[3]	p.o.	2-5 hr	120

(continued)

/1/ After steam sterilization. /2/ Approximately. /3/ 5% solution in fuel oil.

Animal	Dose	mg/kg	Route	Time of Death	Reference
Rabbit	LD	130-160[1]	p.o.	10-16 hr	120
Rabbit	LD	70-85[2]	p.o.	3-6 hr	120
Rabbit	LD	60-70[3]	c.t.	1½-4 hr	120
Rabbit	LD	90-100[4]	c.t.	1½-3 hr	120
Rabbit	LD	40-50[5]	c.t.	9-22 hr	120

PHYTOTOXICITY Highly toxic to foliage and other plant parts [95, 138, 180].

COMPARATIVE TOXICOLOGY Pentachlorophenol does not allow the superficial growth of Aspergillus and Penicillium, as does copper [314].

USE Protectant of materiel: leather, paint, paper, plastics, textiles, wood [111]. Used extensively as protective coating for camouflage materiel. Also used medicinally; agriculturally [180].

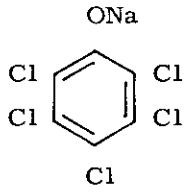
CAUTION Oil solution may cause rapid deterioration of rubber [180].

136. PHENOL, PENTACHLORO-, SODIUM DERIVATIVE

ALTERNATIVE NAMES Pentachlorophenol, sodium salt; Sodium pentachlorophenate.

MOLECULAR FORMULA $C_6Cl_5O{\cdot}Na$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Buff-colored flakes or powder. Molecular weight, 288.342. Decomposes, >300°C. Specific gravity, 1.987 (25/25°C), 1.981 (25/4°C). pH of saturated solution, 10.1 [68]; pH of 1% solution of pure salt, approximately 9 [203]. Soluble (g/100 g solvent at 25°C) in acetone, 37.0; amyl acetate, 97.1; butyl "Cellosolve," 96.4; diacetone alcohol, 46.7; dibutyl phthalate, 18.3; diethylene glycol, 16.4; dipropylene glycol, 74.3; ethyl alcohol (formula 30), 64.0; ethylene glycol, 42.7; methanol, 21.7; methyl ethyl ketone, 94.6; propylene glycol, 70.2; triethylene glycol, 3.4; water, 33; water at 80°C, 39.0. Insoluble in linseed oil, pine oil, soybean oil, Stoddard's solvent, toluene, turpentine, VMP naphtha.

/1/ 11% solution in olive oil. /2/ 5% solution in olive oil. /3/ 5% solution in fuel oil. /4/ 5% solution in "furnace" oil. /5/ 1.8% solution in pine oil.

TESTS *In vitro.*

	Concentration % for Inhibition	% for Kill
Rhizopus nigricans	0.054	0.054
Rhizoctonia solani	0.0022	0.0022
Chaetomium globosum	0.0038	0.0035
Hormiscus gelatinosum	0.011	0.02
Polyporus tulipiferous	0.0022	0.0038
Aspergillus flavus	0.0054	0.011
Lenzites trabea	0.0022	0.0022
Ceratostomella pilifera	0.0038	0.0038
Trichophyton interdigitale	0.0011	0.0011
T. rosaceum	0.0054	0.11
Poria luteofibrata		0.0027

[68]

	Concentration ppm for Total Inhibition
Hormiscus gelatinosum	20
Poria incrassata	20
Trametes serialis	10
Lenzites trabea	20
Chaetomium globosum	60
Aspergillus niger	80
Rhizopus nigricans	40

[181]

Aspergillus niger (Van Tiegham): 0.015% concentration of test compound in medium (yeast extract, peptone, glucose, potassium monophosphate, at pH 6-7), incubated 48 hours at 37°C. Inhibited growth. [291]

In vivo. *Phomopsis citri* and *Diplodia natalensis* (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 2% solution of test compound, dried, and stored 3 weeks at 70°F. Decay prevented; slight rind injury. [181]

TOXICITY *Man.* In 2 reported fatalities, both individuals developed high fever, followed by muscular contractions and death within 24 hours [101].

136. PHENOL, PENTACHLORO-, SODIUM DERIVATIVE (Concluded)

Animals.

Animal	Dose	mg/kg	Route	Time of Death	Reference
Dog	MLD	135	s.c.		120
Guinea pig	MLD	266[1]	c.t.		203
Mouse	MLD	56	s.c.		120
Rabbit	MLD	550	p.o.		120
Rabbit	MLD	218[2]	p.o.		203
Rabbit	MLD	257[1]	c.t.		203
Rabbit	MLD	512.5	c.t.		120
Rabbit	MLD	257	s.c.		120
Rabbit	MLD	135.5	i.p.		120
Rabbit	LD	7090[3]	p.o.	2-5 hr	120
Rabbit	LD	100-130[4]	p.o.	10-16 hr	120
Rabbit	LD	70-85[5]	p.o.	3-6 hr	120
Rabbit	LD	60-70[3]	c.t.	$1\frac{1}{2}$-4 hr	120
Rabbit	LD	90-100[6]	c.t.	$1\frac{1}{2}$-3 hr	120
Rabbit	LD	40-50[7]	c.t.	9-22 hr	120
Rat	LD_{50}	78[8]	p.o.		120
Rat	LD_{50}	125-200	p.o.		120
Rat	LD_{50}	100	s.t.		47

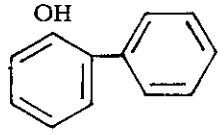
USE Protectant of materiel: paper and wood preservative, slime preventive [111]; mildew control agent, fermentation disinfectant, preservative for paints, adhesives [125].

137. PHENOL, o-PHENYL-

ALTERNATIVE NAMES o-Phenylphenol; Ortho-xenol; o-Hydroxy diphenyl.

MOLECULAR FORMULA $C_{12}H_{10}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Nearly white or light buff crystals [53]. Mild odor. Molecular weight, 170.200. Melting point, 56°C [118], 56-58°C [53], 56.8°C [228], 57°C [180]. Boiling point, 280-284°C; 285.9°C [228], 286°C [180]. Specific gravity, 1.217 (25/25°C) [180]. Vapor pressure, approximately 1 mm Hg (100°C);

/1/ 2% solution in water. /2/ 2% solution in 1% sodium chloride. /3/ 5% solution in fuel oil. /4/ 11% solution in olive oil. /5/ 5% solution in olive oil. /6/ 5% solution in "furnace" oil. /7/ 1.8% solution in pine oil. /8/ Approximately.

volatile in steam [180]. Soluble (g/100 g solvent at 25°C) in acetic acid, >110; acetone, >127; benzene, >106; chloroform, >70.9; diethyl ether, >178; ethanol, >291; ethylene glycol, 234; n-heptane, 4.6; isopropyl alcohol, 587; methanol, 975; neat's-foot oil, 22; olive oil, 50; pine oil, 257; toluene, >125; water, <0.006. [318]

TESTS In vitro. Spores of Stemphylium sarcinaeforme, and Monilinia fructicola: LD_{50}, approximately 50 μg/sq cm [133].

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	Trace	8	63
	100	100	Trace	84	62
	100	100	100	Trace	78

x 10^{-5} M	10	7.5	5.0
% inhibition	85	81	69

250 ppm inhibited growth 100%. [228]

In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 1% solution of test compound, dried, and stored 3 weeks at 70°C. Decay prevented; moderate rind injury.

TOXICITY Man. Moderately toxic. 5% oil solution tolerated on skin, but aqueous solutions of the sodium salt are irritating in concentrations greater than 0.5%. [101] No absorption by skin [325].

Animals. Concentrated solutions in volatile solvents markedly irritating to skin [325] 2.48 g/kg in diet of white rats for 2 years had no adverse effects [180]. Dogs given 0.5 g/kg/da for 1 year showed no effects [325].

Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), and Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight; exposure 22 hours. Caused death.

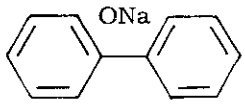
USE Protectant of materiel: textiles, leather, paint finishes [250]. Also used medicinally; agriculturally.

138. PHENOL, o-PHENYL-, SODIUM DERIVATIVE

ALTERNATIVE NAMES o-Hydroxydiphenyl sodium salt; Sodium 2-hydroxydiphenyl; Sodium o-phenylphenate; Sodium o-phenylphenoxide.

MOLECULAR FORMULA $C_{12}H_9O{\cdot}Na$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 192.189. Soluble in water.

TESTS In vitro. Aspergillus niger (Van Tiegham): 0.010% of test compound in nutrient medium (yeast extract, peptone, glucose, potassium dihydrogen phosphate, at pH 6-7); incubated 48 hours at 37°C. Inhibited growth. [181]

In vivo. Phomopsis citri and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in solution of test compound, dried, and stored 3 weeks at 70°F. 5% solution prevented decay; moderate rind injury. 2% prevented decay; slight rind injury. [291]

TOXICITY Animals. LD_{50} in rats, 2.7 g/kg, p.o. [47].

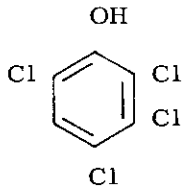
USE Protectant of materiel: textiles, leather [250]; paper [111]; starch [125].

139. PHENOL, 2,3,4,6-TETRACHLORO-

ALTERNATIVE NAME Tetrachlorophenol (2,3,4,6).

MOLECULAR FORMULA $C_6H_2Cl_4O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Brown flakes [53,318]. Strong phenolic odor [318]. Molecular weight, 231.904. Melting point, 56.0°C [318]; 69-70°C [53]; 70°C [228]. Boiling point, 164°C (23 mm Hg) [53]. Specific gravity, 1.839 (24/4°C) [53]. Vapor pressure, approximately 1 mm Hg (100°C). Soluble (g/100 g solvent at 25°C) in acetone, 570; benzene, 189; carbon tetrachloride, 31; diacetone alcohol, 426; ether, 412; ethyl alcohol, 292; fuel oil, No. 2, 35; linseed oil, 40; methanol, 319; mineral

oil, light, 9; neat's-foot oil, 84; pine oil, 203; soybean oil, 92; Stoddard's solvent, 20; toluene, 175; turpentine, 42. [318]

TESTS In vitro. Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.2	1.0	0.9
% inhibition	100	100	100	100	100	100	100

x 10^{-5} M	6.0	5.0	4.0	3.0	2.5	2.0	1.2	1.0	0.5	0.1
% inhibition	100			100			61			
	100	100	Trace	Trace		Trace		57	44	25
		92			91			60	53	32
		91			87			33	30	30

250 ppm inhibited growth 100%. [228]

TOXICITY Man. Skin irritation [53]. Skin absorption [53, 325].

Animals. Dust in atmosphere irritating to nose and throat. Eye contact may cause marked irritation, depending on concentration. [325]

Animal	Dose	mg/kg	Route	Reference
Guinea pig	LD_{50}	250	p.o.	325
Rabbit	LD_{50}	250	Skin absorption	325
Rat	MLD	210[1]	s.c.	120
Rat	LD_{50}	140[1]	p.o.	120

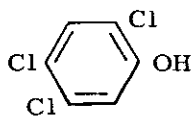
USE Protectant of materiel: textile preservative; preventive of mold growth in paints and cutting oils. Also used medicinally.

140. PHENOL, 2,4,5-TRICHLORO-

ALTERNATIVE NAME 2,4,5-Trichlorophenol.

MOLECULAR FORMULA $C_6H_3Cl_3O$

STRUCTURAL FORMULA



/1/ 4% solution in fuel oil.

140. PHENOL, 2,4,5-TRICHLORO- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Gray flakes in sublimed mass. Strong phenolic odor. Molecular weight, 197.455. Melting point, 60°C [228], 61-63°C [53]. Boiling point, 252°C. Specific gravity, 1.678 (25/4°C). Soluble in alcohol, ether, acetone. [53]

TESTS In vitro. Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.2	1.0	0.9	0.6	0.3	0.12
% inhibition	100	100	100	100	100	100	100	100	100	55

x 10^{-5} M	5.0	4.0	3.0	2.5	2.25	1.0	0.9	0.5	0.45	0.1	0.09
% inhibition	100	100	100	100	Trace	49	49	31	30	13	17
	100				Trace	50	49	35	27	16	20

250 ppm inhibited growth 100%. [228]

TOXICITY Man. Probable LD, 50-500 mg/kg [101]. May cause conjunctivitis, severe lacrimation [250]; skin irritation [53].

USE Protectant of materiel: leather, adhesives, glues, paints, latexes [125]; textiles [111].

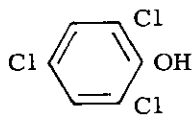
CAUTION Avoid prolonged or repeated contact with compound [228].

141. PHENOL, 2,4,6-TRICHLORO-

ALTERNATIVE NAMES Omal; 2,4,6-Trichlorophenol; sym.-Trichlorophenol.

MOLECULAR FORMULA $C_6H_3Cl_3O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow flakes [53], or rhombic needles [118]. Molecular weight, 197.455. Freezing point, 61°C [53], 62°C [228]. Melting point, 68°C [118]. Boiling point, 244.5°C [118], 248-249°C [53], 252°C [228]. Specific gravity, 1.675 (25/4°C) [53], 1.490 (75/4°C) [118]. Soluble in acetone, alcohol, ether [53].

141. PHENOL, 2,4,6-TRICHLORO- (Concluded)

TESTS In vitro. Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.2	1.0	0.9	0.6	0.3	0.12
% inhibition	100	100	100	100	100	100	100	100	86	45
	100				100	100	100	100	100	53

x 10^{-5} M	5.0	4.5	4.0	3.0	2.25	1.0	0.9	0.5	0.45	0.1	0.09
% inhibition	100	100	100	100	Trace	48	5.1	27	26	15	18

250 ppm inhibited growth 100%. [228]

TOXICITY Man. May cause skin irritation [53].

Animals. LD_{50} in rats (20% solution in fuel oil), 820 mg/kg, p.o.; 2260 mg/kg, s.c. [120]

USE Protectant of materiel: wood [125] and textile preservative [111]. Agricultural.

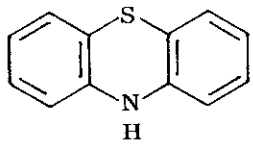
CAUTION Avoid prolonged or repeated contact [228].

142. PHENOTHIAZINE

ALTERNATIVE NAMES Dibenzo-1,4-thiazine; Thiodiphenylamine; Phenthiazine.

MOLECULAR FORMULA $C_{12}H_9NS$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow rhombic leaflets [118]. Molecular weight, 199.266. Melting point, 180°C [118], 185°C [179]. Boiling point, 371°C with decomposition [118]. Soluble in acetone, benzene. Slightly soluble in alcohol, ether. Insoluble in water, chloroform. Oxidizes in presence of air and light [179].

TESTS In vitro. Chaetomium globosum: Spore suspension on fabric impregnated with test compound (4% dry weight) on nutrient agar; incubated 1-3 weeks at 30°C. Compound prevented growth of organism. [70]

142. PHENOTHIAZINE (Concluded)

TOXICITY Man. Probable LD, 500-5000 mg/kg [101]. Gastrointestinal and skin irritation; liver and kidney damage [71]. Overdosage has caused hemolytic anemia, toxic hepatitis, skin photosensitization, pruritus [101].

Animals. LD_{50} in rats, 5000 mg/kg, p.o. [120]. Rats fed diet containing 0.25-0.35% of compound for 125 days, showed no significant changes in blood. [171] MLD in rabbits, 4000 mg/kg, p.o. [120]. Single oral doses (400-2400 mg/kg) caused temporary secondary anemia in rabbits [171].

USE Agricultural [179].

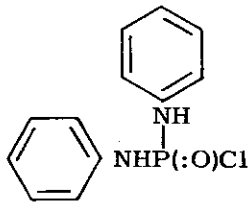
CAUTION Handlers should wear protective clothing [250].

143. PHOSPHORODIAMIDIC CHLORIDE, N,N'-DIPHENYL-

ALTERNATIVE NAME Diamidophosphoryl chloride, N,N'-diphenyl-.

MOLECULAR FORMULA $C_{12}H_{12}ClN_2OP$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 266.664.

TESTS In vitro. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: 1000 µg/sq cm completely stopped spore germination [55].

TOXICITY Mice (27-37 g): LD_{50}, 50 mg/kg, i.v. [11].

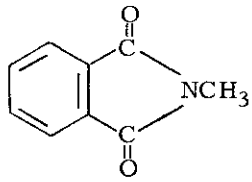
USE Agricultural.

144. PHTHALIMIDE, N-METHYL-

ALTERNATIVE NAME N-Methylphthalimide.

MOLECULAR FORMULA $C_9H_7NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals. Molecular weight, 161.154. Soluble in acetone. Slightly soluble in alcohol. Insoluble in water.

TESTS In vitro.

	µg/sq cm	% Inhibition
Sclerotinia fructicola (Wint.) Rehm.	1000	88
	100	0
	10	0
	1	0
Stemphylium sarcinaeforme Cav.	1000	34
	100	0
	10	0
	1	0

[55]

TOXICITY Rats (albino or hooded, 130-200 g): 500 mg/kg, s.t., non-toxic [296].

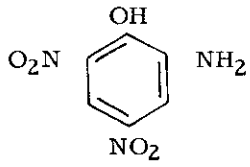
USE Agricultural.

145. PICRAMIC ACID

ALTERNATIVE NAME 2-Amino-4, 6-dinitrophenol.

MOLECULAR FORMULA $C_6H_5N_3O_5$

STRUCTURAL FORMULA



145. PICRAMIC ACID (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Red crystals. Molecular weight, 199.124. Melting point, 168-169°C [118], 168-170°C [228]. Refractive index, 1.54. Soluble in alcohol, ether, benzene, glacial acetic acid, aniline. [118]

TESTS In vitro. 10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 10 ppm. Sclerotinia fructicola: MED, 100 ppm. [55]

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	69 99	64	58	48	24

[228]

Organism	% Inhibition Test Compound, M/L				
	0.001	0.0001	0.00005	0.00001	0.000005
Aspergillus niger	100	33	20	12	5
Penicillium citrinum	28	17	3	0	0
Trichoderma sp	58	14	6	0	-1

[228]

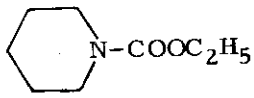
USE Protectant of materiel.

146. 1-PIPERIDINECARBOXYLIC ACID, ETHYL ESTER

ALTERNATIVE NAME Pentamethylene urethane.

MOLECULAR FORMULA $C_8H_{15}NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 157.208. Boiling point, 130°C (20 mm Hg). Miscible with propylene glycol.

146. 1-PIPERIDINECARBOXYLIC ACID, ETHYL ESTER (Concluded)

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm.: 1000 µg/sq cm completely stopped spore germination. Stemphylium sarcinaeforme Cav.: 1000 µg/sq cm did not inhibit spore germination. [55]

Aspergillus niger: 250 ppm inhibited growth 13% [229].

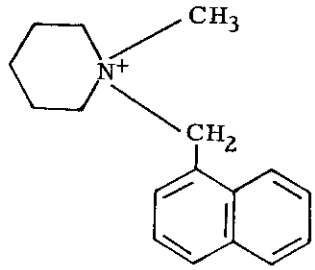
TOXICITY Compound administered to mice, i.p., in gum acacia suspension: Splenic or hepatic emaciation, and severe atrophy, produced by >100 mg/kg; LD_{50}, 250 mg/kg. [266]

USE Agricultural.

147. PIPERIDINIUM IODIDE, 1-METHYL-1-(1-NAPHTHYLMETHYL)-

MOLECULAR FORMULA $C_{17}H_{22}N^{+}\cdot I^{-}$

STRUCTURAL FORMULA



I

PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 367.264. Melting point, 206°C.

TESTS In vitro. Sporotrichum schenckii: North's gelatin agar, seeded with 3×10^7 spore concentration. Aqueous solutions of test compound decreased infestation.

Compound Concentration, %	Zone of Inhibition, mm
3	16
1	11
0.3	7.5
Control	0

[221]

147. PIPERIDINIUM IODIDE, 1-METHYL-1-(1-NAPHTHYLMETHYL)- (Concluded)

Candida albicans: 0.1 ml of a 24-hour culture inoculated into nutrient-Difco broth. 0.3 ml of test compound solution added to triplicate tubes after autoclaving; water control.

Compound Concentration, %	Growth, mm
0.18	?
0.06	0
0.018	3
Control	5

[221]

USE Medicinal.

148. POTASSIUM IODIDE

MOLECULAR FORMULA KI

PHYSICAL AND CHEMICAL PROPERTIES White crystals, granules or powder. Strong, bitter, saline taste. [53] Molecular weight, 166.010. Melting point, 678-705°C [273], 723°C [53]. Specific gravity, 3.123 [53], 3.13 [118]. Refractive index, 1.677. Soluble in water, alcohol, glycerol. [53] Slightly deliquescent in moist air; on long exposure to air, compound becomes yellow due to liberation of iodine. Light and moisture accelerate decomposition. [192]

TOXICITY Man. Vomiting, collapse and coma [71]; coryza, sneezing, lacrimation, swelling of eyelids, metallic taste, gastrointestinal upsets, iodide acne and other eruptions [273].

Animals. LD in rats, approximately 285 mg/kg, i.v. [120].

149. 1,3-PROPANEDIONE, 2-BROMO-1,3-DIPHENYL-

ALTERNATIVE NAME Bromo dibenzoyl methane.

MOLECULAR FORMULA $C_{15}H_{11}BrO_2$

151. PYRIDINE, 3-(HYDROXYMERCURI)-, STEARATE (Concluded)

Organism	Cotton Duck % Original Strength		
	Compound Concentration, %		
	0.05	0.1	0.2
Pestalozzia SN-8	101	111	95
Stachybotrys sp	102	104	83
Thielavia 46	95	104	88
Trichoderma 29	12	89	101
Trichoderma 43	104	106	96

[15]

Aspergillus niger (Van Tiegham): Test compound added to spore suspension in nutrient-toxic-agar; incubated 96 hours at 30°C. Growth completely inhibited by 1×10^{-4} M concentration. [229]

A. niger (Van Tiegham):

$\times 10^{-5}$ M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	71	20

250 ppm inhibited growth 100%. [228]

TOXICITY Man. Tests indicate compound is reasonably well tolerated in ointment form and when impregnated in fabric (concentrations up to 1% in cotton sheeting applied as patches for 48-72 hours) [314].

USE Protectant of materiel: textiles, paints [111, 229].

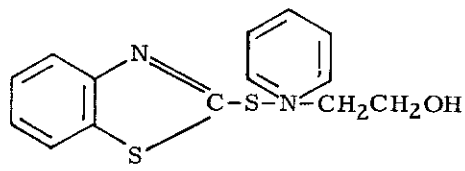
CAUTION Avoid contact with skin and mucous membranes. [228]

152. PYRIDINIUM 2-BENZOTHIAZOLYL SULFIDE, 1-(2-HYDROXYETHYL)-

ALTERNATIVE NAME 2-Mercaptobenzothiazole, β-hydroxyethyl pyridinium salt.

MOLECULAR FORMULA $C_{14}H_{14}N_2OS_2$

STRUCTURAL FORMULA



152. PYRIDINIUM 2-BENZOTHIAZOLYL SULFIDE, 1-(2-HYDROXYETHYL)- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 290.400. Very soluble in water. Insoluble in hydrocarbons. Miscible with small percentage of ether, acetone, alcohol; excess may cause precipitation. Stable at boiling and at melting points.

TESTS In vitro. Stemphylium sarcinaeforme Cav.: Spore germination stopped by 100 μg/sq cm. Sclerotinia fructicola (Wint.) Rehm.: Spore germination stopped by 1 μg/sq cm. [55]

	% for Inhibition	% for Kill
Aspergillus niger	> 0.01	0.02
Chaetomium globosum	0.005	0.01
Myrothecium verrucaria	0.005	0.01
Penicillium sp	> 0.005	0.01

[305]

TOXICITY Man. Not a sensitizer or primary irritant when in contact with skin [305].

Animals. Non-toxic to warm-blooded animals [305]. Mice: 500 mg/kg, in solution of propylene glycol, i.p. daily for 5 days, produced prostration [260].

Salmo trutta (brown trout), Lepomis macrochirus (bluegill sunfish), and Carassius auratus (goldfish): 2 fish each species; test compound concentration, 5 ppm by weight; exposure 24 hours. No injury. [297]

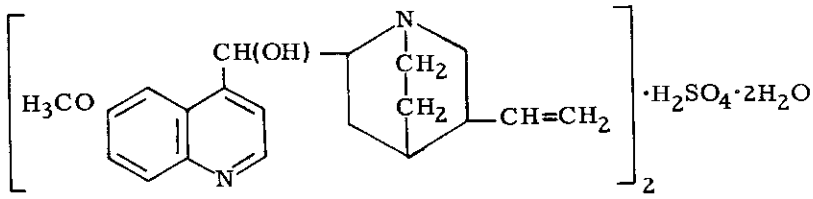
USE Protectant of materiel.

153. QUININE HEMISULFATE, MONOHYDRATE

ALTERNATIVE NAME Quinine sulfate.

MOLECULAR FORMULA $(C_{20}H_{24}N_2O_2)_2 \cdot H_2SO_4 \cdot 2H_2O$

STRUCTURAL FORMULA



153. QUININE HEMISULFATE, MONOHYDRATE (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White, needle-like crystals. Odorless. [53, 260] Very bitter taste [302]. Molecular weight, 782.930. Melting point, 205°C. Soluble in hot water, alcohol. Slightly soluble in chloroform, ether. Turns brown in light. Saturated solution neutral or slightly alkaline to litmus [260].

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 130 μg/sq cm completely inhibited spore germination [140].

TOXICITY Man. Malaise, nausea, vomiting, diarrhea, skin rash, tinnitus, impairment of vision [201].

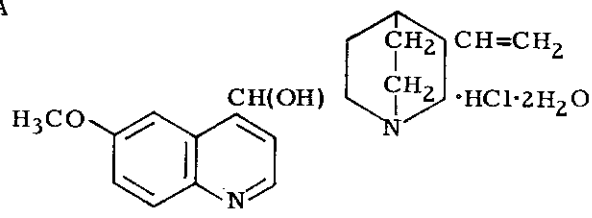
USE Medicinal [302].

154. QUININE, MONOHYDROCHLORIDE, DIHYDRATE

ALTERNATIVE NAME Quinine hydrochloride.

MOLECULAR FORMULA $C_{20}H_{24}N_2O_2 \cdot HCl \cdot 2H_2O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White, amorphous powder or silky needles [192, 254]. Odorless. Bitter taste. [302] Molecular weight, 396.905. Melting point, 156-160°C [254]. Soluble in water, alcohol, glycerin, chloroform. Very slightly soluble in ether. [302]

TESTS In vitro. Sclerotinia fructicola (Wint.) Rehm., and Stemphylium sarcinaeforme Cav.: 130 μg/sq cm completely inhibited growth of spores [140].

154. QUININE, MONOHYDROCHLORIDE, DIHYDRATE (Concluded)

TOXICITY Animals.

Animal	Dose	mg/kg	Route	Time of Death
Cat	MLD	100	s.c.	
Dog	LD	180[1]	s.c.	
Guinea pig	MLD	300	p.o.	4-5 hr
Guinea pig	MLD	160	s.c.	
Guinea pig	LD	293	s.c.	
Rabbit	LD	800	p.o.	7-9 hr
Rabbit	LD	1500[2]	p.o.	
Rabbit	LD	231	s.c.	
Rabbit	LD	250	s.c.	2 hr[1]
Rabbit	LD	500[2]	s.c.	
Rabbit	LD	70[2]	i.v.	
Rat	MLD	<500	p.o.	
Rat	MLD	200	s.c.	
Rat	LD	790	s.c.	
Rat	MLD	300	i.m.	
Rat	MLD	<75	i.v.	
Rooster	LD	857[3]	p.o.	
Frog	MLD	200	s.c.	
Frog	MLD	700	s.c.	
Frog	LD	200	s.c.	
Frog	LD	400	s.c.	
Frog	LD	600[2]	s.c.	

[120]

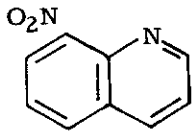
USE Medicinal.

155. QUINOLINE, 8-NITRO-

ALTERNATIVE NAME 8-Nitroquinoline.

MOLECULAR FORMULA $C_9H_6N_2O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Monoclinic needles [118]. Molecular weight, 174.154. Melting point, 89°C [118], 88-92°C [228]. Soluble in alcohol, acetone, ether, benzene. Very slightly soluble in water.

/1/ Approximately. /2/ Hydrobromide. /3/ Hydrochloride.

155. QUINOLINE, 8-NITRO- (Concluded)

TESTS *In vitro*. Test compound placed in depression slide cavity; incubated over night at 25°C with an added spore suspension of 2 x 10^4 cells. *Stemphylium sarcinaeforme* Cav.: 130 µg/sq cm partially inhibited spores. *Sclerotinia fructicola* (Wint.) Rehm.: 130 µg/sq cm completely inhibited germination. [140]

Aspergillus niger (Van Tiegham): 250 ppm inhibited spore germination in nutrient-toxic-agar by 57%; evaluation time, 96 hours [229].

TOXICITY Mice (Banks strain): MTD, 62.5 mg/kg, i.p., in ½% carboxy methyl cellulos [260].

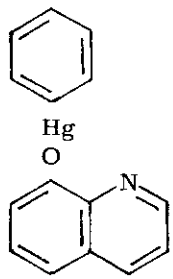
USE Protectant of materiel.

156. QUINOLINE, 8-(PHENYLMERCURIOXY)-

ALTERNATIVE NAME Phenylmercuric 8-hydroxyquinolate.

MOLECULAR FORMULA $C_{15}H_{11}HgNO$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow-orange crystals [193,269]. Molecular weight, 421.856. Melting point, 156-158°C [228], 156-159°C [193], 157-159°C [269]. Soluble in morpholine, hot benzene, ethylene chlorhydrin, acetic acid, dioxane, alcohol, chlorobenzene. Insoluble in hot water, glycerin, isopropyl ether. Stable at pH 2-10. [193]

TESTS *In vitro*. *Aspergillus niger* (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	100	100

[193,269]

156. QUINOLINE, 8-(PHENYLMERCURIOXY)- (Concluded)

Alternari solani spores:

ppm	Mean % Inhibition
100	100
10	100
5	100
2.5	100
1	44
0.5	26
0.1	0

[193, 269]

TOXICITY Mice: Compound administered i.p., daily for 5 days.

mg/kg/da	Mortality
125	3/3
62.5	3/3
31.25	3/3
15.6	2/3
7.8	1/3
3.9	1/3

[261]

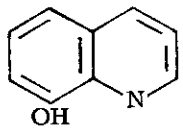
USE Protectant of materiel.

157. 8-QUINOLINOL

ALTERNATIVE NAMES Oxine; 8-Hydroxyquinoline; 8-Quinolinone.

MOLECULAR FORMULA C_9H_7NO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White (pure), tan (tech.), crystals or powder [53, 222]. Phenolic odor. Molecular weight, 145.154. Melting point, 73-75°C [53], 76°C [118, 222]. Boiling point, 267°C [53], 266.9°C [118], 276°C [222]. Soluble in dilute alkalies. Slightly soluble in ether. Very slightly soluble in water. [118] Darkens with exposure to light [53].

157. 8-QUINOLINOL (Concluded)

TESTS In vitro.

	% for Inhibition	% for Kill
Aspergillus ustus	0.01	0.01
Chaetomium globosum	0.001	0.05
Myrothecium verrucaria (Metarrhizium glutinosum)	0.005	0.005

Aspergillus niger, Penicillium sp, Myrothecium verrucaria (Metarrhizium glutinosum), and Chaetomium globosum: 1.53% of test compound on cotton fabric prevented growth. Compound was readily removed by leaching for 24 hours, but even at concentration of 0.01%, growth of C. globosum was inhibited. [314]

Aspergillus niger:

x 10^{-5} M	7.5	5.0	4.0	3.0	2.0	1.0
% inhibition	42	31	73	40	100	0

[228]

TOXICITY Injection in animals caused marked stimulation of the central nervous system. LD_{20} in guinea pigs, 1200 mg/kg, p.o. [120]

PHYTOTOXICITY Non-toxic to plants.

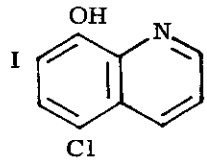
USE Protectant of materiel: paper [111]. Medicinal: dermatomycoses [222]. Agricultural [138].

158. 8-QUINOLINOL, 5-CHLORO-7-IODO-

ALTERNATIVE NAME Iodochlorohydroxyquinoline.

MOLECULAR FORMULA C_9H_5ClINO

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow-brown needles [10]. Slight odor [53]. Molecular weight, 305.505. Melting point, 177-178°C [10]. Soluble in hot glacial acetic acid. Very slightly soluble in water. [10]

158. 8-QUINOLINOL, 5-CHLORO-7-IODO- (Concluded)

TESTS *In vitro*. *Aspergillus niger* (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	100	100	100	77	37

[10,46]

TOXICITY LD_{70} in guinea pigs, 200 mg/kg, p.o. [47]

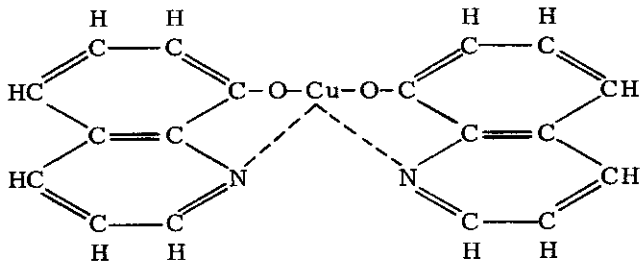
USE Protectant of materiel. Medicinal [10].

159. 8-QUINOLINOL, COPPER (II) DERIVATIVE

ALTERNATIVE NAMES Copper oxinate; Copper-8-quinolinate.

MOLECULAR FORMULA $C_{18}H_{12}N_2O_2Cu$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Yellow-green powder. Odorless. [53] Molecular weight, 351.832. Does not melt. Slightly soluble in pyridine, quinoline. Very slightly soluble in carbon tetrachloride. Practically insoluble in water, common organic solvents, alcohol, ether. [53,318]

TESTS *In vitro*. Malt-agar petri dish test:

	Compound	
	% for Inhibition	% for Kill
Penicillium sp	0.001	
Aspergillus niger	0.05	
A. ustus	0.05	0.05
Chaetomium globosum	0.001	0.05
Myrothecium verrucaria	0.20	0.20
Metarrhizium sp	0.001	
Trichophyton interdigitale	0.001	

[20]

159. 8-QUINOLINOL, COPPER (II) DERIVATIVE (Concluded)

In vivo. Phomopsis citri, and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 5% solution of test compound, dried, and stored 3 weeks at 70°F. Decay prevented; moderate rind injury. [291]

TOXICITY Man. Probable LD, 5-15 g/kg. No skin irritation nor corrosive action when ingested. [101] Patch tests made on 200 individuals showed that test compound is not a primary skin irritant or sensitizer [20].

Animals. MLD in rats, 10 g/kg, p.o. 1 g/kg, administered p.o. to rabbits 2 or 3 days a week until 23 doses had been administered, produced no signs of intoxication and no histological changes in body tissues could be discovered. [20]

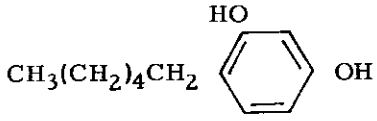
USE Protectant of materiel: canvas [125]; leather, paper, plastics, textiles[1] [111, 227]; wood, rope [227]. Agricultural: apple scab [188, 314]. Medicinal.

160. RESORCINOL, 4-HEXYL-

ALTERNATIVE NAME n-Hexyl resorcinol.

MOLECULAR FORMULA $C_{12}H_{18}O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless needles. Molecular weight, 194.264. Melting point, 68-70°C. Very soluble in alcohol, ether, acetone. Soluble in benzene. Slightly soluble in petroleum ether. [118]

TESTS In vitro. Stemphylium sarcinaeforme spores: LD_{50}, 8 μg/sq cm. Monilinia fructicola spores: LD_{50}, 4.0 μg/sq cm. [138]

TOXICITY Man. Probable LD, 500-5000 mg/kg. Large doses by mouth cause irritation and erosion of gastric and intestinal mucosa. High concentrations irritating to skin. [101] Irritating to mouth, throat, stomach; may injure heart and liver [190].

/1/ About 1% of compound, based on weight of the finished goods, is recommended [20].

Animals. Systemic symptoms are unusual, but damage to liver and heart in dogs has been reported [101].

Animal	Dose	mg/kg	Route
Guinea pig	LD_{50}	475[1]	p.o.
Mouse	MLD	750-1000[2]	s.c.
Mouse	MLD	50[3]	i.p.
Mouse	MLD	200[2]	i.p.
Rat	MLD	250[4]	p.o.
Rat	LD_{50}	550	p.o.

[120]

COMPARATIVE TOXICOLOGY Less toxic than phenol [101].

USE Protectant of materiel: paper preservative [111].

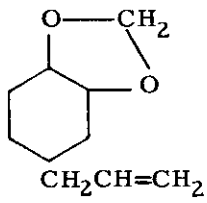
161. SAFROLE

ALTERNATIVE NAME 4-Allyl-1, 2-methylenedioxybenzene.

SOURCE Sassafras or camphor oils.

MOLECULAR FORMULA $C_{10}H_{10}O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless or pale yellow oil. Odor of sassafras. [53] Molecular weight, 162.180. Melting point, 11°C [53]. Boiling point, 233°C [53], 232-234°C [192]. Specific gravity, 1.100-1.107 (15°C) [53], 1.096 (20°C) [192]. Refractive index, 1.5363-1.5385. Soluble in alcohol, ether, benzyl benzoate, fixed oils, mineral oils, chloroform. Slightly soluble in propylene glycol. Insoluble in water, glycerin.

/1/ 25% solution in oil. /2/ 5% solution in olive oil. /3/ 1% water emulsion. /4/ 25% water emulsion.

161. SAFROLE (Concluded)

TESTS *In vitro*. *Sclerotinia fructicola* (Wint.) Rehm.: 1000 μg/sq cm inhibited growth 86% [55].

TOXICITY *Animals*. 2 fish each species; test compound concentration, 5 ppm by weight; exposure 24 hours. *Salmo trutta* (brown trout): Death in <22 hours. *Lepomis macrochirus* (bluegill sunfish), *Carassius auratus* (goldfish): Inactive. [261]

MLD in rabbits, approximately 1000 mg/kg, p.o. or s.c.; 200 mg/kg, i.v. [120]

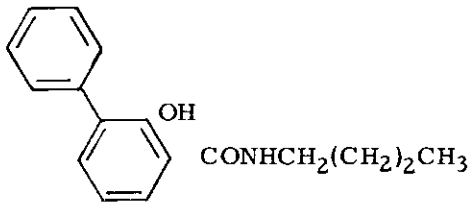
USE Medicinal.

162. SALICYLAMIDE, N-BUTYL-3-PHENYL-

ALTERNATIVE NAME N-Butyl-3-phenyl salicylamide.

MOLECULAR FORMULA $C_{17}H_{19}NO_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 269.330.

TESTS *In vitro*. Sabouraud's agar; both spores and mycelial inoculum employed. Test compound prepared in propylene glycol; incubated 14 days at 30°C. Minimum concentration for inhibition of growth: *Trichophyton (gypseum) mentagrophytes* (Robin) Blanchard, 12 μg/ml; *T. (purpureum) rubrum* (Castellani) Sabouraud, *T. faviforme*, 6 μg/ml; *T. tonsurans*, 3 μg/ml; *Microsporum canis*, 12 μg/ml; *M. fulvum*, 6 μg/ml; *M. audouini* Gruby, 3 μg/ml; *Epidermophyton floccosum* (Harz) Langeron and Milochevitch, 0.8 μg/ml; *Sporotrichum schenckii*, >50 μg/ml. [137]

Minimum inhibitory concentration of test compound in different media: Sabouraud's agar, *Trichophyton (gypseum) mentagrophytes*, 12.0 μg/ml. Tripticase soy broth, *Microsporum audouini* Gruby, 3.0 μg/ml; *Streptomyces sp*, 50.0 μg/ml. Littman oxgall agar, *Aspergillus niger* (Van Tiegham), *Candida albicans*, *Penicillium sp*, >125.0 μg/ml; *Saccharomyces cerevisiae*, *Blastomyces dermatitidis*, >100.0. [137]

TOXICITY Rats: >2000 mg/kg, i.p., caused death in 48 hours [47].

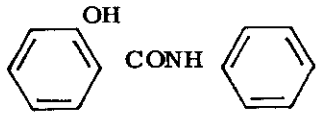
USE Medicinal.

163. SALICYLANILIDE

ALTERNATIVE NAME n-Phenylsalicylamide.

MOLECULAR FORMULA $C_{13}H_{11}NO_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Cream-colored powder [180]; white leaflets [192], prisms or needles [118]. Odorless. Molecular weight, 213.226. Melting point, 134-135°C [53], 135°C [8, 180]. Specific gravity, 2.5. Soluble (g/100 ml solvent at 25°C) in acetone, 47; acetic acid, 4.86; benzene, <0.04; chloroform, <0.03; mineral oil, 0.04; toluene, 1.3; water, <0.02. [180] Stable to air. Compatible with waxes and aluminum salts. pH of saturated solution, 5.74. [53]

TESTS In vitro. In organic coatings, 10% of test compound (based on solids) is required. Up to 2% in waxes, tested with a mixture of Penicillium luteum, Trichoderma sp, Aspergillus niger, and A. flavus, gave poor results. 2-3% proved effective against A. niger.

10-fold dilutions of test compound added to spore suspension in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [53]

Stemphylium sarcinaeforme spores: approximately 10 μg/sq cm. Monilinia fructicola: approximately 3.0 μg/sq cm. [138]

Aspergillus niger (Van Tiegham): 0.25% of test compound in nutrient medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7); incubated 48 hours at 37°C. Inhibited growth. [181]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard: 2,500,000 conidia per plate; Sabouraud's dextrose agar plus horse serum. 1 ml of 0.1% of alcohol solution of test compound in agar; incubated 5 days at 28-30°C. Decreased infestation. Agar disks cut from 15-day culture, immersed 1 minute in 1% solution of test compound, rinsed, and subcultured on Sabouraud's medium for 21 days. Growth not abolished. [312]

Cladosporium herbarum: Satisfactory control in tent calico obtained by immersing material in solution of test compound ($1\frac{1}{2}$ oz/1 gal water). Treatment prevented all but a trace of fungal deterioration at end of 1 year's exposure under very exacting conditions; same conditions produced heavy infection of untreated control within 3-4 months.

Chaetomium globosum: Growth inhibited in 8-oz cotton duck by 0.02-0.04% of test compound. Leaching in static or running water required higher concentration (0.4-0.8%) for inhibition. Aspergillus niger: Growth on fabric inhibited by 0.01-0.02%. [314]

In vivo. 5% of test compound in ointment effective against Microsporum audouini, M. canis, Trichophyton mentagrophytes, T. rubrum, Epidermophyton floccosum [273].

163. SALICYLANILIDE (Concluded)

TOXICITY Man. No skin absorption, no secondary poisoning[325]. May cause irritation and produce inflammation, both beneficial in the treatment of tinea capitis [273].

Animals. LD_{50} in rats, >2.0 g/kg, p.o. Contact with eye caused slight irritation and transient corneal injury in rats. Only slight irritation with prolonged skin contact. [62] Leather treated with 0.25-0.50% of compound safe to use on horses and dogs. [174]

COMPARATIVE TOXICOLOGY Salicylanilide has approximately 8 times the fungistatic power of undecylenic acid against Microsporum audouini [222].

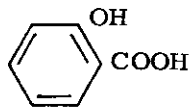
USE Medicinal: ringworm of the scalp [111]. Protectant of materiel: textiles, varnish, leather [53,314]. Agricultural [180].

164. SALICYLIC ACID

ALTERNATIVE NAMES o-Hydroxybenzoic acid.

MOLECULAR FORMULA $C_7H_6O_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White needle-like crystals, or powder. Sweetish, afterward acrid taste. [53] Molecular weight, 138.118. Melting point, 158-161°C [53], 157-159°C [290], 159°C [118]. Boiling point, approximately 211°C (20 mm Hg) [53]. Specific gravity, 1.443 [118], 1.483 [47]. Soluble in acetone, oil of turpentine, alcohol, benzene, ether. Very slightly soluble in water. Stable in air, but gradually discolored by light. [53]

TESTS In vitro. Aspergillus niger (Van Tiegham): 0.13% of test compound in nutrient medium (yeast extract, peptone, glucose, potassium phosphate, at pH 6-7); incubated 48 hours at 37°C. Inhibited growth. [181]

Trichophyton (gypseum) mentagrophytes (Robin) Blanchard: 2,500,000 conidia per plate; Sabouraud's dextrose agar, plus 10% horse serum; 1 ml of 0.1% alcohol solution of test compound in agar; incubated 5 days at 28-30°C. Decreased infestation. Agar disks from 15-day culture in 1% solution of test compound immersed 1 minute, rinsed, and subcultured on Sabouraud's medium 21 days. Did not abolish growth. [312]

Stemphylium sarcinaeforme spores: LD_{50}, approximately 5 μg/sq cm. Monilinia fructicola spores: LD_{50}, approximately 50 μg/sq cm. [138]

Aspergillus niger:

ppm	% Inhibition
250	29
50	2
25	0

[228]

A. niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% Inhibition	30	20	12	-1	-2

[228]

Organisms susceptible in vitro: Epidermophyton floccosum (Harz) Langeron and Milochevitch, Malassezia furfur, Microsporum audouini Gruby, M. canis Bodin, M. gypseum (Bodin) Guiart and Grigorakis, Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, T. rubrum, T. (Achorion) schoenleinii (Lebert) Langeron and Milochevitch, T. (endodermophyton) concentricum Blanchard, T. violaceum.

TOXICITY Man. Irritating to skin [222]. Marked irritant to gastrointestinal tract. [273]

Animals.

Animal	Dose	mg/kg	Route	Reference
Cat	LD_{50}	400[1]	p.o.	47
Dog	MLD	450-500[2]	p.o.	120
Dog	LD	300-400[2]	s.c.	120
Dog	LD	991	i.p.	120
Guinea pig	MLD	850	s.c.	120
Guinea pig	MLD	900[2]	i.p.	120
Mouse	LD_{50}	480	p.o.	47
Mouse	LD_{60}	520	s.c.	120
Rabbit	LD	1100-1600	p.o.	47
Rat	LD_{50}	900	p.o.	47
Rat	MLD	700	s.c.	120
Frog	MLD	500-900	s.c.	120

USE Medicinal [99]. Protectant of materiel: textiles, paper [111].

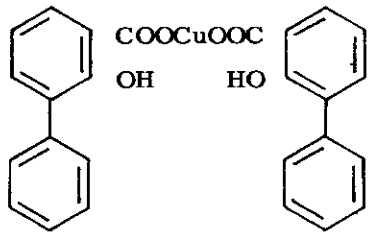
/1/ Approximately. /2/ Sodium salt.

165. SALICYLIC ACID, 3-PHENYL-, COPPER (II) SALT

ALTERNATIVE NAME Copper-3-phenyl salicylate.

MOLECULAR FORMULA $C_{26}H_{18}O_6Cu$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Tan crystals. Odorless. [318] Molecular weight, 489.944. Decomposes, 148-152°C [179]. Non-volatile [318]. Moderately soluble in acetone, acetophenone, amyl acetate, n-butyl oleate, chlorobenzene, cottonseed oil, dibutyl phthalate, dioxane, ethylene dichloride, linseed oil, methyl n-amyl ketone, olive oil, phenyl n-butyl ketone, pine oil, propylene glycol, toluene, trichloroethylene, xylene. Practically insoluble in water [318].

TESTS In vitro. Aspergillus niger:

ppm	% Inhibition
250	87
100	66
50	59, 48

[228]

Organism	% Inhibition			
	Test Compound, M/L			
	0.002	0.001	0.0001	0.00001
Aspergillus niger	100	100	69	
Trichoderma sp		100	71	29
Trichoderma T-1	100	100	79	
Penicillium citrinum		100	27	14

[228]

TOXICITY Man. Probable LD, 500-5000 mg/kg. No skin irritation or absorption; little or no corrosive action when ingested. [101] 0.5-3% concentrations impregnated in textiles produced no skin irritation or sensitization [250].

Animals. LD_{50} in rats, 520 mg/kg, p.o. 0.1% fed in diet to rats for 4 months had no ill effects; 0.3% had minimal effects. [325]

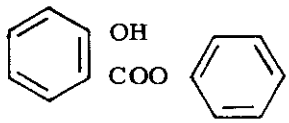
USE Protectant of materiel: textiles [111, 250].

166. SALOL

ALTERNATIVE NAME Phenyl salicylate.

MOLECULAR FORMULA $C_{13}H_{10}O_3$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals or crystalline powder. Aromatic odor. [192] Molecular weight, 214.210. Melting point, 43°C [99], 41-43°C [192]. Boiling point, 173°C (12 mm Hg). Specific gravity, 1.25. [118] Very soluble in ether, benzene, chloroform, acetone, oils. Very slightly soluble in glycerol.

TESTS In vitro. 10-fold dilutions of test compound added to spore suspension in depression slide cavity. Stemphylium sarcinaeforme Cav.: 10,000 ppm did not inhibit germination. Sclerotinia fructicola (Wint.) Rehm.: 1000 ppm inhibited germination. [55]

Monilinia fructicola spores: LD_{50}, approximately 50 µg/sq cm. Stemphylium sarcinaeforme, >1000 µg/sq cm. [138]

TOXICITY Man. Probable LD, 50-500 mg/kg [111].

COMPARATIVE TOXICOLOGY Toxic effects similar to those of phenol, but without phenol's marked corrosive action on the alimentary tract [111].

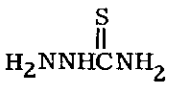
USE Protectant of materiel: paper [111]. Medicinal [99, 118].

167. SEMICARBAZIDE, 3-THIO-

ALTERNATIVE NAME Thiosemicarbazide.

MOLECULAR FORMULA CH_5N_3S

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystalline powder [53, 192]. Molecular weight, 91.140. Melting point, 180-184°C. Soluble in water, alcohol. [53]

TESTS In vitro. Cryptococcus hominis: 0.04% of test compound in aqueous solution (40 mg/L) added to nutrient medium (Sabouraud's dextrose-peptone-agar plates); incubated 7 days. Growth completely inhibited. [275]

Aspergillus niger: 250 ppm inhibited growth 7%.

TOXICITY

Animal	LD_{50}, mg/kg	Route
Cat	20	s.t.
Dog	10	s.t.
Guinea pig	24	i.p.
Rat	11	s.t.
Rat	18	s.t.
Rat, Alexandrine	23	s.t.
Rat, cotton	16	s.t.
Rat, wild Norway, young	19	s.t.
Rat, wild Norway, adult	13	s.t.

[47]

USE Protectant of materiel.

168. SODIUM AZIDE

MOLECULAR FORMULA NaN_3

PHYSICAL AND CHEMICAL PROPERTIES Colorless or white, hexagonal crystals or leaflets. Molecular weight, 65.021. Decomposes, approximately 300°C [53]. Specific gravity, 1.846 [118]. Soluble in water. Slightly soluble in alcohol, benzene. Slightly alkaline pH because of hydrolysis.

TESTS In vitro. Saccharomyces carlsbergensis: 5×10^{-5} M of test compound inhibited growth [232].

Aspergillus niger:

ppm	% Inhibition
25	100
10	89
5	66
1	21

[228]

168. SODIUM AZIDE (Concluded)

TOXICITY LD_{50} in mice, 19 mg/kg, i.v.; 28-34 mg/kg, i.p. [47] Test compound dissolved in normal saline: LD_{50} in mice, 26.5 mg/kg, i.p.; LD_{10}, 23.2 mg/kg, i.p. [282] Test compound in suspension or solution (0.25% agar or aqueous saline): LD_{50} in albino mice, 51 mg/kg [217].

USE Protectant of materiel.

169. SODIUM CHROMATE

MOLECULAR FORMULA Na_2CrO_4

PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals [118]. Molecular weight, 162.004. Specific gravity, 2.710 (36°C). Soluble in water. Slightly soluble in alcohol. [118]

TOXICITY Man. Probable LD, 50-500 mg/kg. If ingested, circulatory collapse and toxic nephritis may result. [101]

Animals.

Animal	Dose	mg/kg	Route	Time of Death	Reference
Dog	LD	145.8-162	i.v.	78 min	120
Guinea pig	LD	20-30	s.c.		120
Mouse	MTD	62.5	i.p.		261
Rabbit	LD	243	s.c.	45 min	120
Rabbit	LD	97-162	i.v.	5-7 hr	120
Rabbit	LD	19.4-32	i.v.	2-4 da	120

USE Protectant of materiel.

170. SODIUM FLUORIDE

MOLECULAR FORMULA NaF

PHYSICAL AND CHEMICAL PROPERTIES Clear, lustrous crystals, or white powder or balls [53]. Molecular weight, 41.997. Melting point, 980-997°C [118], 993°C [53]. Specific gravity, 2.766. Soluble in water. Slightly soluble in alcohol [53].

170. SODIUM FLUORIDE (Concluded)

TOXICITY Man. Probable LD, 50-500 mg/kg. Sublethal: nausea, vomiting, abdominal distress, diarrhea, stupor, weakness. Lethal: muscular weakness, tremors, convulsions, collapse, respiratory and cardiac failure. Chronic: mottling of tooth enamel, osteosclerosis.

Animals.

Animal	Dose	mg/kg	Route	Reference
Cat	LD	13.7	s.c.	120
Dog	MLD	50-100	p.o.	120
Dog	MLD	80	i.v.	120
Dog	MLD	31-50	i.m.	120
Dog	LD	150-160	s.c.	120
Guinea pig	MLD	250	p.o.	120
Guinea pig	MLD	400	s.c.	120
Mouse	LD	80	p.o.	120
Mouse	LD	70	s.c.	120
Mouse	LD	125	i.p.	120
Rabbit	MLD	100-200	p.o.	120
Rabbit	MLD	200	p.o.	120
Rabbit	LD	87.5	i.v.	120
Rat	MLD	125	s.c.	120
Rat	MLD	28-35	i.p.	120
Rat	LD_{50}	250	p.o.	47
Rat	LD_{50}	180	p.o.	47
Rat	LD_{50}	200	p.o.	120
Rat	LD_{50}	40	i.p.	47
Frog	MLD	400	s.c.	120

PHYTOTOXICITY Highly toxic to plants [180].

USE Protectant of materiel: wood [99]; paper, wool [111].

CAUTION Avoid breathing dust [53].

171. SORBIC ACID

ALTERNATIVE NAMES Hexadienic acid; 2,4-Hexadienic acid.

MOLECULAR FORMULA $C_6H_8O_2$

STRUCTURAL FORMULA $CH_3CH{:}CHCH{:}CHCOOH$

171. SORBIC ACID (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White crystalline solid [53]. Molecular weight, 112.124. Melting point, 134.5°C [53,118]. Boiling point, 120°C (10 mm Hg) [118]; 228°C, with decomposition [231]. Vapor pressure, <0.01 mm Hg (20°C). Very soluble in alcohol, ether. Slightly soluble in water. [118]

TOXICITY Man. Probable LD, 5,000-15,000 mg/kg. Not a primary skin irritant or sensitizing agent. [101] May cause corneal burns [250].

Animals. Rats: LD_{50}, 10.5 g/kg, p.o. 5.06 g/kg/da in diet for 90 days, caused extensive liver damage; 2.48 g/kg/da had no effect.

Rabbits: 5% of test compound in propylene glycol caused severe eye injury. 1% caused minor injury. Powder applied to the eye in excess, caused severe transient injury. 10% in acetone (belly vesicant test) did not cause irritation. [205]

USE Protectant of materiel [205].

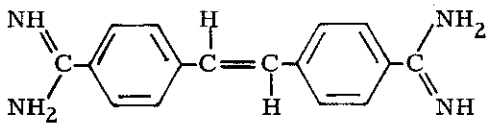
CAUTION Handlers should wear chemical safety goggles [250].

172. 4,4'-STILBENEDICARBOXAMIDINE

ALTERNATIVE NAMES Stilbamidine; 4,4'-Diamidinostilbene.

MOLECULAR FORMULA $C_{16}H_{16}N_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystalline powder [117]. Molecular weight, 264.320. Decomposes, 290°C. Slightly soluble in water, methyl alcohol. [120]

TESTS In vivo. North American blastomycosis: Test compound effective in 42 out of 51 cases (disappearance of active lesions and demonstrable organisms). As little as 0.9 g effective in 1 child.

TOXICITY Man. Local irritation, vascular reactions, kidney and liver damage, delayed facial neuropathy from trigeminal lesions [117].

Animals. LD_{50} in mice, 43-53 mg/kg, i.p. LD_{50} in hamsters, 50 mg/kg, i.p. [120]

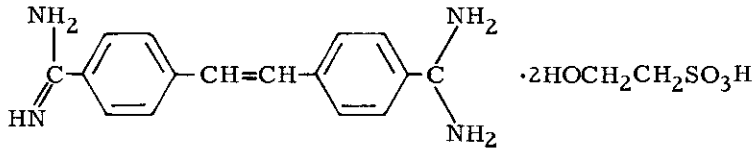
USE Medicinal: deep mycoses [67].

173. 4,4'-STILBENEDICARBOXAMIDINE, DIISETHIONATE

ALTERNATIVE NAME 4,4'-Diamidinostilbene, isethionate.

MOLECULAR FORMULA $C_{16}H_{16}N_4 \cdot 2C_2H_6O_4S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White, crystalline powder. Odorless. [46] Molecular weight, 516.588. Decomposes, 325-335°C. Freely soluble in water. Very slightly soluble in alcohol. Practically insoluble in ether. [46] Darkens above 250°C; discolored by light. Stable in air; unstable in alkaline or neutral solution.

TESTS In vitro. Organisms susceptible: Blastomyces dermatitidis, Coccidioides immitis, Histoplasma capsulatum.

TOXICITY Man. Local irritation, vascular reactions, kidney and liver damage, delayed facial neuropathy from trigeminal lesions. Paresthesia and anesthesia in forehead reported. Readily absorbed from gastrointestinal tract and parenteral sites of administration. Maximum blood levels achieved within 30 minutes; only about 10% excreted. [105]

COMPARATIVE TOXICOLOGY Most toxic of the diamidine compounds [105].

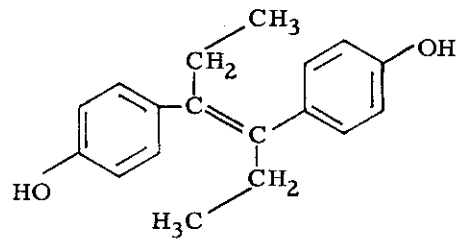
USE Medicinal: intermediate and deep mycoses [192, 252, 273].

174. 4,4'-STILBENEDIOL, α,α'-DIETHYL-

ALTERNATIVE NAMES Stilbestrol; α,α'-Diethylstilbenediol; 3,4-Bis(p-hydroxyphenyl)-3-hexene; 4,4'-Dihydroxy-α,β-diethylstilbene; Diethylstilbestrol.

MOLECULAR FORMULA $C_{18}H_{20}O_2$

STRUCTURAL FORMULA



174. 4,4'-STILBENEDIOL, α,α'-DIETHYL- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White crystalline powder. Odorless. [53] Molecular weight, 268.340. Melting point, 169-172°C. Soluble in alcohol, ether, chloroform, fatty oils, dilute hydroxides, vegetable oils. Almost insoluble in water. [53, 192] Sensitive to light [8]. Neutral to litmus.

TOXICITY Man. Nausea, vomiting, and headache [8].

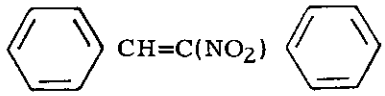
Animals. Mice: 2500-5000 mg/kg, p.o., in sesame oil, produced death in 1 hour. 500-1000 mg/kg, s.c., death in 10-16 days. [120]

USE Medicinal.

175. STILBENE, α-NITRO-

MOLECULAR FORMULA $C_{14}H_{11}NO_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 225.236.

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 75 ppm inhibited growth 100%. [211]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav., and Sclerotinia fructicola (Wint.) Rehm.: MED, 10 ppm. [211]

TOXICITY Mice, injected i.p.:

mg/kg	Mortality
500	5/5
250	0/3
125	0/3
62.5	0/3
31.3	0/3

[261]

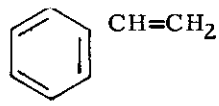
USE Protectant of materiel.

176. STYRENE

ALTERNATIVE NAMES Vinyl benzene; Phenylethylene; Cinnamene; Styrol; Styrolene.

MOLECULAR FORMULA C_8H_8

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless [53], oily [192], liquid [53,72]. Penetrating [192], aromatic [53] odor. Molecular weight, 104.064. Freezing point, -30.628°C [72]. Boiling point, 145.20°C [72], 146°C [118]. Vapor pressure, 0.656 mm Hg (25°C) [72]. Specific gravity, 0.906 [72], 0.9074 [118]. Refractive index, 1.5462 [72], 1.54344 (17°C) [118]. Miscible with alcohol, ether, acetone, carbon tetrachloride, n-heptane, benzene. Very slightly soluble in water. [72] Polymerization and oxidation with exposure to light and air [192].

TOXICITY Man. Apparent CNS depression. Moderately irritating to skin and mucous membranes. [65] May cause dilated pupils [253].

Animals. LD_{50} in rats, 5000 mg/kg, p.o. [47].

Guinea pigs and rats (continuous exposure to lethal concentrations of test compound):

LC_{100}, mg/L	ppm	Time of Death
6.0-6.3	1300	40 hr
9.3	2000	30 hr
11.6	2500	21 hr
23.2	5000	8 hr

[120]

USE Protectant of materiel.

CAUTION Avoid prolonged contact with skin. Vapor harmful. [53] Fire hazard [250].

177. SUCCINIC ACID, ALKENYL-, MONOBUTYL ESTER, MERCURY SALT

MOLECULAR FORMULA $C_xH_xO_4 \cdot Hg$

PHYSICAL AND CHEMICAL PROPERTIES Brown, resinous liquid. Soluble in benzene.

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 250 ppm inhibited growth 100%.

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 10 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 100 ppm. [4]

TOXICITY Animals. May cause dyspnea and hypersensitivity [261]. Mice, injected i.p.:

mg/kg	Mortality
6.25	0/3
12.5	0/3
25	1/3
50	2/3
100	3/3
200	3/3

[261]

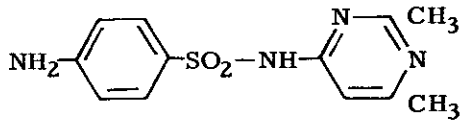
USE Protectant of materiel.

178. SULFANILAMIDE, N^1-(2,6-DIMETHYL-4-PYRIMIDINYL)-

ALTERNATIVE NAMES Elkosin; 6-Sulfanilamido-2,4-dimethylpyrimidine.

MOLECULAR FORMULA $C_{12}H_{14}N_4O_2S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 278.330. Melting point, 240-242°C [124]. Soluble in 200 mg/100 ml water at 37°C [6].

178. SULFANILAMIDE, N^1-(2,6-DIMETHYL-4-PYRIMIDINYL)- (Concluded)

TESTS *In vivo*. Mice infected intraperitoneally with *Nocardia asteroides*, and *Candida albicans*, in 4% gastric mucin. Suspension of test compound given orally 1 hour before infection and continued daily in 2 equally divided doses for 5 days. Mice were observed for 21 days.

Mice	mg/kg[1]	Average Survival Time da
Nocardia asteroides infected		
Lot A	2500	17.8
Lot B	1250	18.1
Lot C	500	18.1
Lot D	250	19.9
Controls		6.2
Candida albicans infected		
Lot A	2500	21
Lot B	1250	21
Controls		0.8

[88]

TOXICITY *Man*. Low incidence of nausea, vomiting, rash, fever, hematuria or marke leukopenia [198]. Rare kidney damage, bone marrow damage, hemolytic anemia, CNS an gastrointestinal disturbances, methemoglobinemia [71].

Animals. LD_{50} in mice, 1776 mg/kg, i.v. [47].

COMPARATIVE TOXICOLOGY Of any single sulfa drug, test compound involves least risk of urolithiasis [322].

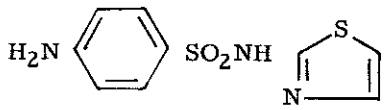
USE Medicinal.

179. SULFATHIAZOLE

ALTERNATIVE NAMES 2-Sulfonaminothiazole; p-Aminobenzene-sulfonamidothiazole.

MOLECULAR FORMULA $C_9H_9N_3O_2S_2$

STRUCTURAL FORMULA



/1/ Twice daily.

179. SULFATHIAZOLE (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White or faintly yellow crystals or powder [53]. Odorless, or nearly so [105]. Molecular weight, 255.318. Melting point, 200-204°C. Soluble in acetone, dilute mineral acids, or aqueous solutions of potassium and sodium hydroxide. [53] Soluble (mg/100 ml) in water, 96 (pH 5.5); urine, 100 (pH 5); serum, 250-330; alcohol, 525. [105] Light sensitive [302].

TOXICITY Man. Fever, maculopapular rash, pruritis, chills, malaise, headache [105]. Fever, hematuria, anuria, skin lesions, painful joints, acute leukopenia with granulocytopenia, interference with muscular contraction, neuritic pains [201].

Animals.

Animal	Dose	mg/kg	Route	Reference
Mouse	LD_{50}	6000	p.o.	5
Mouse	LD_{50}	4500[1]	p.o.	120
Mouse	LD_{50}	1450-1950	s.c.	120
Mouse	LD_{50}	1700	s.c.	5
Mouse	LD_{50}	990[1]	i.v.	120
Rat	LD_{100}	1250	i.p.	120

USE Medicinal: epidermophytosis of feet, groin, axilla, hands [67, 201].

180. SULFIDE, BIS(DIMETHYLTHIOCARBAMYL)-

ALTERNATIVE NAME Tetramethylthiuram monosulfide.

MOLECULAR FORMULA $C_6H_{12}N_2S_3$

STRUCTURAL FORMULA

$$(CH_3)_2NC(=S)SC(=S)N(CH_3)_2$$

PHYSICAL AND CHEMICAL PROPERTIES Yellow crystals [159]. Molecular weight, 208.370. Melting point, 103.5-103.7°C [207], 103-104°C [159], 109-110°C [78]. Soluble in alcohol, acetone, benzene, chloroform [207]. Slightly soluble in ether [228]. Insoluble in water, gasoline [207]. Stable in dilute alkalies [228].

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 250 ppm inhibited growth 100%. [78, 207]

/1/ Sodium salt.

180. SULFIDE, BIS(DIMETHYLTHIOCARBAMYL)- (Concluded)

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 10 ppm. [78, 207]

Aspergillus niger:

x 10^{-4} M	10	7.5	5.0	2.5	1.0
% inhibition	100	100	98	71	21

[228]

TOXICITY Man. Irritating to nose and throat membranes [250].

Animals. Male mice, given single i.p. injection of compound dissolved in water or propylene glycol; observation period 10 days:

mg/kg	Mortality
350	10/10
300	8/10
250	3/10
200	0/10

[280]

USE Protectant of materiel.

CAUTION Avoid inhalation.

181. SULFIDE, DODECYL PHENYLMERCURI- [1]

ALTERNATIVE NAME Phenylmercuric-tert.-dodecyl mercaptide.

MOLECULAR FORMULA $C_{18}H_{30}HgS$

STRUCTURAL FORMULA

PHYSICAL AND CHEMICAL PROPERTIES Viscous liquid [85]. Molecular weight, 479.096. Melting point, <25°C (crude). Insoluble in water. Stable at room temperature. [85]

/1/ Mixture of tert.-dodecyl isomers.

181. SULFIDE, DODECYL PHENYLMERCURI- (Concluded)

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours. 250 ppm inhibited growth 100%. [85]

TOXICITY Mice, injected i.p.:

mg/kg	Mortality
500	3/3
250	3/3
125	3/3
62.5	3/3
31.3	1/3
15.7	0/3

[261]

USE Protectant of materiel.

CAUTION Avoid skin contact.

182. SULFONE, BIS(2-CHLOROETHYL)-

MOLECULAR FORMULA $C_4H_8Cl_2O_2S$

STRUCTURAL FORMULA $(ClCH_2CH_2)_2SO_2$

PHYSICAL AND CHEMICAL PROPERTIES Colorless crystals. Molecular weight, 191.084. Melting point, 57°C. Boiling point, 230°C. Vapor pressure, 7.2 mm Hg x 10^{-8} (0°C), 8.8 mm Hg x 10^{-6} (20°C), 0.0018 mm Hg (50°C). Soluble in water (hydrolyzes slightly), alcohol, olive oil, glacial acetic acid, ether, chloroform, benzene.

TESTS In vitro. Aspergillus niger (Van Tiegham): 250 ppm in nutrient-toxic-agar, incubated 96 hours at 30°C. Growth inhibited 100%. [229]

TOXICITY

Animal	mg/kg[1]	Route	Time of Death
Mouse	35[2]	s.c.	15 da
Mouse	50[2]	i.v.	15 da
Rat	50[2]	s.c.	15 da
Rat	>72	i.v.	15 da

[47]

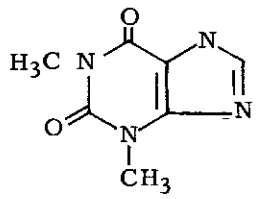
USE Medicinal.

/1/ In propylene glycol. /2/ Approximately.

183. THEOPHYLLINE

MOLECULAR FORMULA $C_7H_8N_4O_2$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Monoclinic needles [118]. Odorless. Bitter taste. [250] Molecular weight, 180.166. Melting point, 260-272°C. Soluble in ether, alkalies, ammonium hydroxide. [118] Slightly soluble in water, alcohol [53].

TESTS In vitro. Ophiostoma multiannulatum: Conidia and test compound in nutrient medium. 0.2-0.5% of test compound decreased growth; 0.6% completely inhibited growth.

TOXICITY Man. Highly toxic. Principal manifestations: collapse, fall in blood pressure. [71]

Animals.

Animal	LD, mg/kg	Route
Cat	100[1]	p.o.
Guinea pig	170-200	s.c.
Rabbit	300-400	p.o.
Rabbit	100-130	i.v.

[120]

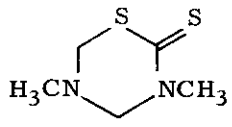
USE Protectant of materiel.

184. 2H-1,3,5-THIADIAZINE-2-THIONE, TETRAHYDRO-3,5-DIMETHYL-

ALTERNATIVE NAMES Tetrahydro-3,5-dimethyl-2H-1,3,5-thiadiazine-2-thione; 3,5-Dimethyltetrahydro-1,3,5-2H-thiadiazine-2-thione.

MOLECULAR FORMULA $C_5H_{10}N_2S_2$

STRUCTURAL FORMULA



/1/ In water.

184. 2H-1,3,5-THIADIAZINE-2-THIONE, TETRAHYDRO-3,5-DIMETHYL- (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES White, crystalline powder. Almost odorless. [179] Molecular weight, 162.278. Melting point, 100-103°C. Soluble (% by weight, at 25°C) in trichloroethane, 26; cyclohexanone, 25; ethylene dichloride, 21; acetophenone, 16; isophorone, 6; water, 0.12 (30°C); acetone, 19.4 (30°C). Stable as dry powder. High temperature and acid solutions speed hydrolytic breakdown. [185]

TESTS In vitro. 0.25% spray ineffective on Rhizopus nigricans; inhibited growth of Monilinia fructicola 63%, with slight injury to some of the fruit. [263]

TOXICITY Man. On 200 subjects, 100 ppm on gauze gave neither primary irritation nor sensitization reactions [205].

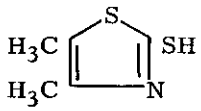
Animals. LD_{50} in mice, 650 mg/kg, p.o. [179]. 15% of test compound in propylene glycol produced very slight eye injury in rabbits [205].

USE Protectant of materiel: paper, leather, glue, casein, starch [53,125]. Agricultural [179]: dry rot in gladioli [53].

185. 2-THIAZOLETHIOL, 4,5-DIMETHYL-

MOLECULAR FORMULA $C_5H_7NS_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 145.246.

TESTS In vitro. Test compound, in acetone or Tween 20, added to Difco malt extract agar at pH 4.6, and sterilized. 15 ml of medium placed in petri dish and seeded with mycelia and/or spores; incubated for 6 days at 20°C.

	Colony Diameter mm	% Response
Fusarium lycopersici Sacc.	35	24
Control	46	
Sclerotinia fructicola (Wint.) Rehm.	3	93
Control	45	
Trichophyton rosaceum (Sab.)	8	47
Control	15	
Phytophthora cinnamoni	0	100
Control	56	
Polyporus tulipiferus	17	76
Control	70	

[260]

185. 2-THIAZOLETHIOL, 4,5-DIMETHYL- (Concluded)

TOXICITY 128 mg/kg/da (in gum acacia suspension), injected i.p. in mice for 7 days, produced death.

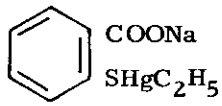
USE Medicinal; agricultural.

186. THIMEROSAL

ALTERNATIVE NAMES Merthiolate; Sodium ethylmercurithiosalicylate; Thiomersalate.

MOLECULAR FORMULA $C_9H_9O_2SHg \cdot Na$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Light-cream, crystalline powder. Slight odor. [53] Molecular weight, 404.835. Soluble in water. Almost insoluble in ether, benzene. Affected by light. [53]

TESTS In vitro. Phomopsis citri, and Diplodia natalensis (stem-end rot in citrus fruit): 25 ethylene gas treated oranges dipped in 0.001% of test compound, dried, and stored at 70°C for 3 weeks. Decay prevented; slight rind injury. [291]

TOXICITY Man. Occasional urticaria, progressing to weeping dermatitis. In rare instances, anemia, leukopenia, liver damage. [71]

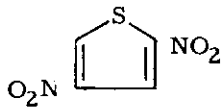
Animals. LD_{50} in mice, 66 mg/kg, s.c.; 45 mg/kg, i.v. [120]

USE Medicinal. Protectant of materiel: control of fungus attack on optical instruments [250].

187. THIOPHENE, 2,4-DINITRO-

MOLECULAR FORMULA $C_4H_2N_2O_4S$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Molecular weight, 174.138. Melting point, 50.4-51.8°C [145].

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

ppm	% Inhibition
250	100
150	100
125	100
75	100
37.5	100

TOXICITY Mice: LD, 1.0 mg/kg, i.p.; MTD, 0.5 mg/kg, i.p. [145]

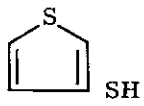
USE Protectant of materiel.

CAUTION Avoid exposure to vapor, or contact with solid [145].

188. 3-THIOPHENETHIOL

MOLECULAR FORMULA $C_4H_4S_2$

STRUCTURAL FORMULA



MOLECULAR WEIGHT 116.204.

TESTS In vitro. Aspergillus niger (Van Tiegham) spores (TC-215-4347 Steinberg): Nutrient-toxic-agar containing test compound inoculated with 1 drop of spore suspension (5 ml in 95 ml distilled water and wetting agent); plates incubated at 30°C. Terminal reading taken at 96 hours.

(continued)

188. 3-THIOPHENETHIOL (Concluded)

x 10^{-4} M	10.0	7.5	5.0	2.5	1.0
% inhibition	92	74	68	57	36

250 ppm inhibited growth 100%. [265]

10-fold dilutions of test compound added to spores in depression slide cavity; incubated 17 hours. Stemphylium sarcinaeforme Cav.: MED, 100 ppm. Sclerotinia fructicola (Wint.) Rehm.: MED, 10 ppm. [265]

TOXICITY Mice, injected i.p.:

mg/kg	Mortality
500	3/3
250	3/3
125	3/3
62.5	1/3
31.25	1/3
15.7	1/3
7.8	0/3

[265]

USE Protectant of materiel.

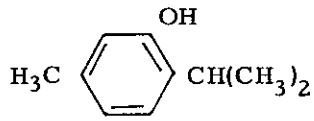
189. THYMOL

ALTERNATIVE NAMES Isopropyl cresol; 5-Methyl-2-isopropylphenol; 3-Hydroxy-p-cymene; Thymic acid; Thyme camphor; 3-p-Cymenol; 3-Hydroxy-1-methyl-4-isopropylbenzene.

SOURCE From the essential oil of Thymus vulgaris or Monorda punctata.

MOLECULAR FORMULA $C_{10}H_{14}O$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystals [53]. Aromatic, pungent, thyme-like odor [301]. Somewhat caustic taste [192]. Molecular weight, 150.212. Melting *point*, 49-51°C [53], 49.6°C [126], 51.5°C [273]. Boiling point, 233°C [53,273]. Specific gravity, 0.979. Soluble in alcohol, carbon disulfide, chloroform, glacial acetic acid, ether, fixed or volatile oils. Slightly soluble in water, glycerol. [53] Affected by light [302].

TESTS In vitro. Trichophyton (gypseum) mentagrophytes (Robin) Blanchard, Microsporum canis Bodin, Sporotrichum schenckii, Blastomyces dermatitidis: Sabouraud's agar streaked with 10-day agar slant culture of test organism; incubated 15 days at 25°C. Growth was inhibited completely by 3.1, 25, 30, and 50 ppm. [195]

TOXICITY Man. Probable LD, 50-500 mg/kg [101]. Nausea, vomiting, depression, mental confusion, temporary deafness, convulsions, cardiac and respiratory collapse [71, 101, 250, 273]. Skin irritant in concentrations higher than 2% [273].

Animals.

Animal	Dose	mg/kg	Route
Cat	MLD	250	p.o.
Guinea pig	MLD	1100	s.c.
Guinea pig	MLD	300	i.p.
Guinea pig	MLD	>2000[1]	i.p.
Mouse	MLD	800	p.o.
Mouse	LD_{50}	1800 ± 224[2]	p.o.
Rabbit	MLD	750-1000	p.o.
Rabbit	MLD	60[1]	i.v.
Rabbit	LD	>2000	s.c.
Rat	MLD	1600-1700	s.c.
Frog	LD	150	s.c.

[120]

COMPARATIVE TOXICOLOGY Resembles phenol in its systemic action, but is less toxic (probably because it is less soluble) [101].

USE Medicinal: superficial mycoses [250, 273]. Protectant of materiel: paper [192].

190. TRICHOMYCIN

SOURCE Streptomyces hachijoensis.

PHYSICAL AND CHEMICAL PROPERTIES Yellow powder. Decomposes, 155°C. Soluble in water, aqueous acetone, aqueous methanol, aqueous ethanol, at slightly alkaline pH. Less soluble in butanol, ethanol, methanol, acetone. Insoluble in ether, petroleum ether, ethyl acetate, amyl alcohol. Thermostable at pH 7-8.5; unstable at pH 2. [121]

TESTS In vitro. Candida albicans, 56 strains: Inhibited by 0.05-0.4 units/ml. Most strains of C. tropicalis, C. krusei inhibited by 2.5-10 μg/ml. C. solani, Torulopsis spp, Saccharomyces carlsbergensis, Hansenula anomala, Rhodotorula mucilaginosa, not sensitive to high concentrations. [121]

/1/ In oil. /2/ In cotton oil.

190. TRICHOMYCIN (Concluded)

In vivo. Candida albicans: 4 i.v. doses of 20 μg/da protected infected mice [121].

TOXICITY Man. 50 mg, p.o., tolerated [121].

Animals. Mice: LD_{50}, 160 mg/kg, s.c.; 4.2 mg/kg, i.p. Oral doses of 160 mg/kg were tolerated, 830 mg/kg were lethal. [121]

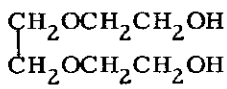
USE Medicinal.

191. TRIETHYLENE GLYCOL

ALTERNATIVE NAME TEG.

MOLECULAR FORMULA $C_6H_{14}O_4$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES Colorless liquid. Practically odorless. [53] Molecular weight, 150.172. Freezing point, -7.2°C. Boiling point, 287.4°C. Specific gravity, 1.1254 (20/20°C). Soluble in water. Immiscible with benzene, toluene, gasoline. [53]

TESTS In vitro. Penicillium notatum: Series of tubes prepared containing 5 cc triethylene glycol-water solutions, ranging from 10-70% at 10% intervals, and from 70-100% at 5% intervals. Each tube was inoculated with the sediment of 1 cc of a 2,500,000 per cc spore suspension, the final spore concentration being 500,000 per cc. Resulting suspensions were thoroughly shaken at frequent intervals, and 0.1 cc removed and plated on Sabouraud's agar at 10-minute, 20-minute, 30-minute, 1-hour, 2-hour, and 5-hour intervals, then daily for 10 days following the time of inoculation. Concentration for shortest killing time, 85%; 25-minute treatment gave 90% kill. [191]

TOXICITY Man. May cause iritis, slight corneal necrosis [250].

Animals. No ill effects from exposure to vapors for 12-18 months, or from repeated oral administration of doses several hundred times greater than those absorbed through the lungs. [105]

191. TRIETHYLENE GLYCOL (Concluded)

Animal	Dose	mg/kg	Route
Guinea pig	LD_{50}	14,000(13,750-15,700)	p.o.
Mouse	LD_{50}	20,913	p.o.
Mouse	LD_{50}	9844	s.c.
Mouse	LD_{50}	7313	i.v.
Mouse	LD	8150	i.p.
Rat	MLD	8400	i.m.
Rat	LD_{50}	22,060(19,380-25,130)	p.o.
Rat	LD_{50}	12,375-16,875	p.o.

[120]

USE Medicinal [53, 191].

192. 10-UNDECENOIC ACID

ALTERNATIVE NAMES Undecylenic acid; 10-Hendecenoic acid; Desenex.

MOLECULAR FORMULA $C_{11}H_{20}O_2$

STRUCTURAL FORMULA $CH_2=CH(CH_2)_8COOH$

PHYSICAL AND CHEMICAL PROPERTIES Colorless to yellow-white to yellow [273], oily liquid [165]. Sweet, fatty odor [252]. Molecular weight, 184.270. Melting point, 20-21°C; decomposes, 275°C. [222] Boiling point, 160°C (10 mm Hg). Specific gravity, 0.910-0.913 (25/25°C). [122] Refractive index, 1.4475-1.4485 (25°C) [53]. Miscible with alcohol, chloroform, ether, benzene, fixed and volatile oils. Insoluble in water. [222] Stable.

TESTS In vitro. Trichophyton (gypseum) mentagrophytes, T. purpureum, Epidermophyton floccosum, Microsporum felineum, Cryptococcus neoformans, Aspergillus fumigatus: 20,000-25,000 ppm killed organisms after 5-minute contact [165].

Trichophyton (gypseum) mentagrophytes: 38 ppm, in Sabouraud's maltose broth. Fungistatic [164].

Stemphylium sarcinaeforme Cav.: 100 µg/sq cm completely stopped spore germination. Sclerotinia fructicola (Wint.) Rehm.: 10 µg/sq cm completely stopped spore germination. [55]

Organisms susceptible in vitro: Candida albicans, Epidermophyton floccosum, Microsporum audouini, M. canis, M. gypseum, Trichophyton (gypseum) mentagrophytes, T. rubrum, T. tonsurans, T. verrucosum, T. violaceum. [222]

TOXICITY Man. Ointment and powder: Side effects negligible in concentrations recommended for therapeutic use (not over 10% when applied to skin, 1% for use on mucous membranes) [273].

Animals. LD_{50} in rats, approximately 1620 mg/kg, p.o. [179]; approximately 2500 mg/kg, p.o. [120].

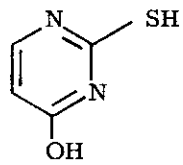
USE Medicinal: superficial mycoses [163, 252, 279]. Agricultural.

193. URACIL, 2-THIO-

ALTERNATIVE NAMES 2-Thio-4-oxypyrimidine; Thiouracil; 2-Mercapto-4-hydroxypyrimidine.

MOLECULAR FORMULA $C_4H_4N_2OS$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White, bulky, crystalline powder. Odorless. Bitter taste. [53] Molecular weight, 128.154. Melting point, 340°C, with decomposition. Slightly soluble in water. Insoluble in alcohol. [53]

TESTS In vitro. Cryptococcus hominis: Test compound, in solution of water and dilute alkali, completely inhibited growth [275].

TOXICITY Man. Leukopenia, granulocytopenia, drug fever, skin eruptions. [192]

Animals. LD_{100} in rats (hooded, Rowelt strain), 20-200 mg/animal, i.p. [163].

USE Medicinal.

194. UREA, THIO-

ALTERNATIVE NAME Thiocarbamide.

MOLECULAR FORMULA CH_4N_2S

STRUCTURAL FORMULA H_2NCSNH_2

PHYSICAL AND CHEMICAL PROPERTIES White lustrous crystals. Bitter taste. Molecular weight, 76.124. Melting point, 182°C. Sublimes in vacuo at 150-160°C. Specific gravity, 1.405 [118], 1.406 [53]. Soluble in cold water, ammonium thiocyanate solution, alcohol. Nearly insoluble in ether. [53]

TESTS In vivo. Phomopsis citri, and Diplodia natalensis (stem-end rot in citrus fruit): 5% gave excellent control; no rind injury. [295]

TOXICITY Man. Repeated use may induce agranulocytosis, thrombopenia. Rapidly excreted unchanged in urine. [101] Nausea, headache, abdominal cramps, skin eruptions, jaundice, arthralgia, hyperpyrexia [155].

Animals. Toxicity in rats varies with species and diet. [120]

Animal	Dose	mg/kg	Route	Reference
Guinea pig	MLD	4000	s.c.	120
Rabbit	MLD	6985	p.o.	120
Rat[1]	MLD	100	s.t.	296
Rat[2]	LD_{50}	1830	p.o.	120
Rat[2]	LD_{50}	1830[3]	s.t.	62
Rat[2]	LD_{50}	1830 ± 135	i.p.	120
Rat[4]	LD_{50}	125-640	p.o.	120
Rat[5]	LD_{50}	4.0 ± 0.2	i.p.	120
Frog	MLD	10,000	s.c.	120

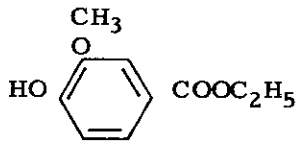
USE Medicinal; agricultural.

195. VANILLIC ACID, ETHYL ESTER

ALTERNATIVE NAME Ethyl 4-hydroxy-3-methoxy benzoate.

MOLECULAR FORMULA $C_{10}H_{12}O_4$

STRUCTURAL FORMULA



/1/ Albino and hooded. /2/ Norway. /3/ In 10% gum acacia. /4/ Domestic. /5/ Hopkins.

195. VANILLIC ACID, ETHYL ESTER (Concluded)

PHYSICAL AND CHEMICAL PROPERTIES Colorless needles [118]. Cinnamon-like taste [73]. Molecular weight, 196.196. Melting point, 44°C. Boiling point, 293°C. Very soluble in alcohol, ether. Soluble in alkalies. Insoluble in water. [118]

TESTS In vitro. Organisms susceptible: Coccidioides immitis, Histoplasma capsulatum [222]. Inhibitory to most pathogenic fungi, including the superficial ones, in concentrations ranging from 100-300 μg/ml [50, 73].

TOXICITY Man. 30,000-45,000 mg/da for 3-18 months produced occasional nausea, acidosis, hyperpnea. Liver and kidney damage from large doses after a month or more. [222]

Animals. LD_{50} in rats, 2000 mg/kg, s.c. MLD in rabbits, 3000 mg/kg in 4-5% solution in milk, p.o. [120] Guinea pigs will tolerate 1000 mg/kg/da, p.o., whereas rabbits can take 3 times as much over a period of several weeks [73].

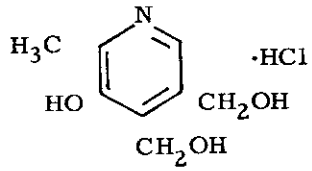
USE Medicinal: histoplasmosis, coccidioidomycosis [73, 222].

196. VITAMIN B_6 HYDROCHLORIDE

ALTERNATIVE NAMES Beadox hydrochloride; 3-Hydroxy-4, 5-dihydroxymethyl-2-methyl-pyridine; Pyridoxine hydrochloride.

MOLECULAR FORMULA $C_8H_{11}NO_3 \cdot HCl$

STRUCTURAL FORMULA



PHYSICAL AND CHEMICAL PROPERTIES White crystalline powder. Odorless. [8] Molecular weight, 205.641. Decomposes, 205-212°C [95]. Soluble in water, 1:5; alcohol, 1:90. Stable in air; slowly affected by sunlight. [8]

TESTS In vitro. Stemphylium sarcinaeforme Cav.: 130 μg/sq cm completely inhibited spore germination. Sclerotinia fructicola (Wint.) Rehm.: 130 μg/sq cm did not inhibit spore germination. [140]

196. VITAMIN B_6 HYDROCHLORIDE (Concluded)

TOXICITY Man. Irritating if injected subcutaneously or intramuscularly [201].

Animals.

Animal	Dose	mg/kg	Route	Time of Death	Reference
Mouse, albino	LD_{50}	1130[1]	i.v.		218
Rat	LD	6000	p.o.	36-72 hr	47
Rat	LD	3700	s.c.	36-72 hr	47

USE Medicinal.

/1/ Single dose.

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APPENDIXES

APPENDIX I. PATENT NUMBERS

Compound	Country	Patent Number	Year
Acetic acid, dichloro-	Germany	246,661	1911
		824,342	1951
Acetophenone, 4'-hydroxy-	U.S.	1,961,630	1934
Acrylonitrile	U.S.	2,356,075	
Ammonium chloride, alkylbenzyldimethyl-	U.S.	2,634,228	1953
Ammonium lactate, tris(2-hydroxy-ethyl)(phenylmercuri)-	U.S.	2,698,263	1954
Antimycin A	U.S.	2,657,170	1953
Antipyrine	Japan	40,194	1921
Benzene, hexachloro-	Germany	729,904	1942
Benzene, (2-nitropropenyl)-	U.S.	2,601,282	1952
Benzoic acid	U.S.	1,284,287	1918
		1,284,888	1918
		1,285,117	1918
		1,332,028	1920
		1,365,956	1921
		1,367,898	1921
		1,458,491	1923
		1,463,190	1923
		1,463,225	1923
		1,557,153	1925
		1,576,999	1926
		1,591,245	1926
		1,787,581	1931
		2,415,800	1947
		2,497,889	1950
		2,561,350	1951
		2,595,181	1952
		2,595,227	1952
		2,662,923	1953
		2,665,280	1954
		2,673,217	1954
	France	379,715	1907
	Germany	175,295	1903
		216,091	1907
		236,489	1910
		261,775	1911
	Great Britain	23,575	1914
		116,348	1917
		119,517	1917
		119,518	1917
		124,605	1918
		132,433	1919
		143,392	1919
		197,319	1923
		578,608	1946
		642,459	1950
		698,157	1953

(continued)

Compound	Country	Patent Number	Year
Benzoic acid (concluded)	Holland	62,757	1949
		64,720	1949
	Japan	2,424	1952
		5,218	1954
	Sweden	140,411	1953
	U.S.S.R.	66,248	1946
p-Benzoquinone	U.S.	1,318,631	1919
		1,322,850	1919
		1,752,293	1930
		2,130,151	1938
		2,144,424	1939
		2,281,327	1942
		2,285,858	1942
		2,343,768	1944
		2,624,747	1953
	Great Britain	556,166	1943
Benzothiazole, 6-(2-diethylaminoethoxy)-2-dimethylamino-, dihydrochloride	U.S.	2,578,757	1951
	Great Britain	667,621	1952
	Japan	2,487	1953
		4,777	1953
		6,286	1953
		2,632	1954
Benzothiazole, 2-mercapto-	U.S.	1,962,109	1934
		2,631,153	1953
		2,666,764	1954
	Austria	8210/32	1933
	Germany	913,173	1954
	Great Britain	407,691	1934
		407,708	1934
		700,339	1953
		717,372	1954
Bicyclo[2,2,1] hept-5-ene-2,3-dicarboximide, 1,4,5,6,7,7-hexachloro-N-(ethylmercuri)-	U.S.	2,598,562	
p,p'-Biphenol	U.S.	2,368,361	1945
4-Biphenylamine	U.S.	2,149,525	1939
		2,400,874	1946
Borax	U.S.	911,695	1909
		1,090,526	1914
		1,450,975	1923
		1,492,920	1924
		1,573,259	1926
		2,105,109	1938
		2,175,178	1939
		2,184,558	1939
		2,333,334	1943
		2,455,595	1948
		2,517,076	1950
		2,517,958	1950

Compound	Country	Patent Number	Year
Borax (concluded)	U.S.	2,528,481	1950
		2,540,648	1951
	Canada	213,223	1931
	France	442,820	1912
	Germany	223,025	1909
	Great Britain	794	1909
		18,764	1910
		4,736	1912
		107,109	1917
		158,992	1919
		175,201	1921
	Holland	71,113	1952
	U.S.S.R.	52,591	1938
		52,592	1938
		57,503	1940
		58,839	1941
Bordeaux mixture	Hungary	119,243	1938
Butyric acid, 3,3-dimethyl-	U.S.	2,004,066	1935
		2,481,159	1949
Captan	U.S.	2,553,770	1951
		2,553,771	
	Great Britain	666,636	1952
Carbamic acid, dimethyldithio-, iron salt	U.S.	1,972,961	1934
		2,614,958	1952
		2,614,960	1952
Carbamic acid, dimethyldithio-, sodium salt	U.S.	2,614,957	1952
Carbamic acid, dimethyldithio-, zinc salt	U.S.	2,229,562	1941
		2,243,161	1948
		2,492,314	1949
		2,614,959	1952
Carbamic acid, ethylenebis(dithio-, disodium salt	U.S.	2,317,765	
Carbamic acid, ethylenebis(dithio-, zinc salt	U.S.	2,317,765	
Carbanilic acid, thiono-, ethyl ester	Japan	179,287	1949
Carvacrol	U.S.	1,449,121	1923
	Canada	188,518	1919
Chloramphenicol	U.S.	2,483,884	1949
		2,483,892	1949
		2,586,661	1952
		2,692,896	1954
	Denmark	78,168	1954
	Great Britain	651,174	1951
		687,749	1953
		692,265	1953
		695,769	1953

(continued)

Compound	Country	Patent Number	Year
Chloramphenicol (concluded)	Great Britain	698,544	1953
		698,808	1953
		701,718	1953
		717,297	1954
	Japan	1,762	1952
		1,765	1952
		4,875	1952
		227	1953
		4,198	1954
	Switzerland	275,968	1951
		282,878	1952
		283,587	1953
Chloranil	U.S.	2,349,771	1944
		2,349,772	1944
		2,414,008	1947
		2,422,089	1947
		2,422,229	1947
		2,519,319	1950
	Italy	415,715	1949
	Japan	3,770	1952
		6,029	1953
	U.S.S.R.	50,439	1937
		50,440	1937
Chloropicrin	U.S.	2,181,411	1940
		2,365,981	1944
	Great Britain	2,387	1908
Chlortetracycline	U.S.	2,482,055	1949
		2,606,329	1952
		2,655,535	1953
		2,709,672	1955
	Great Britain	690,381	1953
		704,079	1954
Citric acid	U.S.	2,066,892	1937
		2,072,919	1937
		2,121,064	1938
		2,148,874	1939
		2,253,061	1941
		2,353,771	1944
		2,362,906	1944
		2,364,701	1944
		2,394,031	1946
		2,400,143	1946
	France	801,273	1936
		802,461	1936
		803,630	1936
		819,173	1937
		819,279	1937
		833,631	1938
	Germany	636,135	1936

Compound	Country	Patent Number	Year
Citric acid (concluded)	Germany	679,847	1939
		680,595	1939
		698,905	1940
	Great Britain	462,350	1937
		474,897	1937
		491,534	1938
		517,793	1940
	Hungary	117,222	1937
	U.S.S.R.	43,649	1935
		57,144	1940
		57,807	1940
		58,981	1941
Cresol	U.S.	2,391,566	1945
		2,417,291	1947
		2,451,996	1948
	Great Britain	580,926	1946
		602,257	1948
		672,512	1952
		701,438	1953
		721,160	1954
	Holland	69,367	1952
	Hungary	128,953	1942
	Italy	443,203	1948
	Japan	180,674	1949
		3,264	1951
m-Cresol	U.S.	1,025,616	1912
		2,439,735	1948
		2,523,707	1950
		2,640,084	1953
		2,662,923	1953
	France	976,578	1951
		976,579	1951
	Germany	247,272	1911
		673,380	1939
	Great Britain	2,458	1912
		3,923	1912
		524,541	1941
		600,839	1948
		695,464	1953
		717,578	1954
	Japan	176,239	1948
o-Cresol	U.S.	2,395,638	1946
		2,401,608	1946
		2,530,369	1950
		2,603,662	1952
		2,678,337	1954
	France	976,578	1951
		976,579	1951
	Great Britain	508,526	1939

(continued)

Compound	Country	Patent Number	Year
o-Cresol (concluded)	Great Britain	600,839	1948
	Japan	176,239	1948
p-Cresol	U.S.	2,533,203	1950
		2,663,735	1953
		2,678,337	1954
		2,683,751	1954
	France	976,578	1951
		976,579	1951
	Great Britain	600,839	1948
		626,095	1949
		684,039	1952
		695,464	1953
		707,006	1954
		717,588	1954
	Japan	176,239	1948
Cyclohexanone	U.S.	2,456,692	1948
		2,552,300	1951
		2,557,281	1951
		2,565,087	1951
		2,684,984	1954
	France	977,009	1951
	Great Britain	649,680	1951
		681,613	1952
		716,820	1954
	Japan	7,219	1951
		6,613	1953
Dehydroacetic acid	U.S.	2,229,204	1941
	Canada	384,872	1939
Dichlone	U.S.	2,302,382	
		2,422,089	
		2,349,771	1944
		2,349,772	1944
		2,422,229	1947
		2,585,229	1952
	Italy	433,853	1948
		433,854	1948
	Japan	1,283	1954
		1,838	1954
Diethylamine, 2,2'-dichloro-N-methyl-, hydrochloride	Austria	167,872	1951
Diphenhydramine hydrochloride	U.S.	2,668,857	1954
	Great Britain	605,915	1948
		606,317	1948
		607,258	1948
		646,048	1950
		679,803	1952
	Holland	74,951	1954

Compound	Country	Patent Number	Year
Diphenhydramine hydrochloride (concluded)	Japan	5,678	1953
Disulfide, bis(diethylthiocarbamyl)-	U.S.	2,375,083	1945
		2,464,799	1949
Disulfide, bis(dimethylthiocarbamyl)-	U.S.	1,876,059	1932
		2,375,083	1945
		2,385,410	1945
		2,461,963	1949
		2,695,881	1954
	Great Britain	374,594	1932
	Holland	71,829	1953
	Italy	440,231	1948
	U.S.S.R.	39,102	1934
		53,766	1938
		56,086	1939
1,2-Dithiolo[4,3-b]pyrrol-5(4H)-one, 6-acetamido-4-methyl-	Great Britain	692,066	1953
	Japan	5,400	1954
Ethane, 1,2-dibromo-	U.S.	2,391,890	1946
Ethane, 1,1,2-trichloro	U.S.	2,174,737	1940
	France	804,491	1936
	Great Britain	461,220	1937
Ethylene oxide	U.S.	20,370	1937*
		2,125,333	1938
		2,136,183	1939
		2,156,341	1939
		2,172,025	1939
		2,177,361	1939
		2,232,910	1941
		2,238,474	1941
		2,241,019	1941
		22,241	1942*
		2,270,780	1942
		2,294,383	1942
		2,366,724	1945
		2,367,169	1945
		2,370,768	1945
		2,371,848	1945
		2,417,685	1947
		2,424,086	1947
		2,430,443	1947
		2,437,930	1948
		2,458,266	1949
		2,463,228	1949
		2,477,435	1949
		2,491,057	1949
		2,554,459	1951
		2,562,857	1951
		2,578,841	1951

(continued)

*Reissue

Compound	Country	Patent Number	Year
Ethylene oxide (concluded)	U.S.	2,585,483	1952
		2,587,468	1952
		2,600,444	1952
		2,628,965	1953
		2,649,463	1953
		2,653,952	1953
		2,680,752	1954
		2,686,762	1954
		2,693,474	1954
	Australia	142,908	1951
	Belgium	425,430	1938
	Canada	387,564	1940
		422,937	1944
		433,589	1946
	France	813,582	1937
		831,547	1938
	Germany	845,937	1952
	Great Britain	466,416	1937
		466,417	1937
		531,256	1944
		558,776	1944
		560,770	1945
		573,545	1945
		587,584	1947
		590,479	1947
		657,165	1951
		676,358	1952
		686,151	1953
		687,243	1953
		704,227	
	Holland	67,215	1951
	Japan	172,936	1946
		176,645	1948
		179,579	1949
Ethylene, tetrachloro-	U.S.	1,590,265	1926
		2,139,219	1938
		2,140,551	1938
		2,178,622	1939
		2,222,931	1940
		2,249,512	1941
		2,255,752	1941
		2,374,923	1945
		2,381,001	1945
		2,417,059	1947
		2,440,768	1948
		2,442,323	1948
		2,442,324	1948
		2,447,410	1948
		2,478,201	1949

Compound	Country	Patent Number	Year
Ethylene, tetrachloro- (concluded)	U.S.	2,525,589	1950
		2,538,723	1951
		2,572,913	1951
		2,577,388	1951
		2,588,867	1952
		2,606,937	1952
		2,610,215	1952
	Austria	162,898	1949
		164,479	1949
		166,909	1950
		167,119	1950
	Belgium	447,012	1942
		447,044	1942
		447,046	1942
		449,037	1943
	France	815,601	1937
		832,749	1938
		832,750	1938
		841,962	1939
	Germany	694,884	1940
		712,579	1941
		725,276	1942
		733,693	1943
		734,024	1943
		734,027	1943
		734,722	1943
		809,812	1951
		818,347	1951
		846,847	1952
	Great Britain	468,921	1937
		480,568	1938
		500,176	1939
		535,026	1941
		575,672	1946
		653,802	1951
		663,364	1951
		671,947	1952
		673,396	1952
		673,565	1952
	Sweden	132,770	1951
	U.S.S.R	50,533	1937
Ethylene, trichloro-	U.S.	2,108,390	1938
		2,140,548	1939
		2,155,723	1939
		2,161,078	1939
		2,181,672	1940
		2,286,985	1942
		2,292,129	1943
		2,319,261	1943

(continued)

Compound	Country	Patent Number	Year
Ethylene, trichloro- (concluded)	U.S.	2,322,258	1944
		2,338,297	1944
		2,361,072	1944
		2,369,485	1945
		2,374,923	1945
		2,378,859	1945
		2,379,372	1945
		2,397,724	1946
	Canada	377,115	1938
		395,846	1941
	France	814,423	1937
		841,728	1939
		854,111	1940
	Germany	171,900	
		263,457	
		649,118	1937
		718,057	1942
		719,914	1942
		721,380	1942
		736,232	1943
	Great Britain	469,573	1937
		473,644	1937
		480,568	1938
		503,644	1939
		503,645	1939
		506,078	1939
		517,213	1940
		523,555	1940
		555,487	1943
		565,494	1944
		575,530	1946
	U.S.S.R.	50,533	1937
Formic acid	U.S.	857,046	1907
		891,793	1908
		960,927	1910
		970,145	1910
		970,825	1910
		975,151	1910
		975,866	1910
		1,043,985	1912
		1,048,609	1912
		1,185,028	1916
		1,235,426	1917
		1,344,851	1920
		1,396,006	1921
		1,522,257	1925
		2,070,503	1937

Compound	Country	Patent Number	Year
Formic acid (continued)	U.S.	2,160,064	1939
		2,196,156	1940
		2,286,407	1942
		2,369,655	1945
		2,390,713	1945
		2,436,804	1946
		2,557,281	1951
		2,645,661	1953
	France	367,316	1906
		382,339	1907
		417,815	1909
		464,608	1913
		819,576	1937
	Germany	182,691	1904
		193,509	1905
		214,155	1906
		209,418	1907
		247,490	1907
		232,707	1908
		235,752	1909
		245,168	1909
		234,580	1910
		239,075	1910
		243,225	1910
		243,797	1911
		288,266	1911
		281,044	1913
		639,064	1936
		677,697	1939
		696,868	1940
		706,576	1941
		710,170	1941
		714,970	1941
		720,013	1942
	Great Britain	14,438	1906
		22,038	1906
		3,428	1908
		20,893	1909
		8,438	1910
		784	1912
		9,762	1915
		110,555	1917
		123,325	1919
		123,326	1919
		198,385	1921
		213,599	1923
		217,467	1923
		217,747	1923
		475,016	1937

(continued)

Compound	Country	Patent Number	Year
Formic acid (concluded)	Great Britain	628,034	1949
		650,126	1951
		728,511	1955
	Norway	34,668	1922
	Switzerland	227,917	1943
Glutarimide, 3-[2-(3-5-dimethyl-2-oxocyclohexyl)-2-hydroxyethyl] -	U.S.	2,574,519	1951
	Great Britain	639,943	1950
2-Imidazoline, 2-heptadecyl-	U.S.	2,540,170	
		2,540,171	
	Great Britain	598,927	
Iodine	Great Britain	6,562	1911
Isothiocyanic acid, allyl ester	Germany	705,651	1941
Menadione	U.S.	2,311,093	1943
		2,319,094	1943
		2,331,725	1943
		2,373,003	1945
		2,392,852	1946
		2,402,054	1946
		2,402,226	1946
		2,525,515	1950
	Germany	714,572	1941
		804,102	1951
	Great Britain	526,927	1940
		574,899	1946
		596,095	1947
		668,494	1952
	Hungary	123,817	1940
		124,314	1940
		135,060	1948
	Japan	162,647	1944
	U.S.S.R.	66,489	1946
Mercury acetate, phenyl-	U.S.	1,786,094	1930
		1,879,206	1932
		2,075,971	1937
		2,366,683	1945
		2,418,986	1947
		2,535,595	1951
		2,686,119	1954
	France	843,092	1939
	Great Britain	325,266	1928
	Japan	2,696	1950
		5,333	1951
		6,950	1951

Compound	Country	Patent Number	Year
Mercury acetate, phenyl- (concluded)	Switzerland	253,422	1948
Mercury (II) chloride	U.S.	1,084,346	1914
		1,312,743	1919
		1,331,690	1920
		1,373,357	1921
		2,517,076	1950
	Germany	258,432	1911
		262,184	1912
		281,842	1914
	Great Britain	19,601	1912
		172,205	1920
	Holland	4,763	1920
		8,480	1922
		75,223	1954
	Italy	430,949	1948
		437,943	1948
	Japan	36,433	1920
	Sweden	50,918	1922
Mercury oleate, phenyl-	Great Britain	585,633	1947
Methane, bromo-	U.S.	2,156,869	1939
		2,244,324	1941
		2,244,341	1941
		2,244,629	1941
	Germany	703,835	1941
DL-Methionine, N-(2-carboxy-ethyl)-	U.S.	2,562,198	1951
1-Naphthol, 2,4-dinitro-	Switzerland	234,830	1949
1,2-Naphthoquinone	U.S.	2,395,638	1946
	Great Britain	508,526	1939
1,4-Naphthoquinone	U.S.	2,373,003	1945
		2,395,638	1946
		2,585,229	1952
	France	949,465	1949
	Great Britain	508,526	1939
2-Norpinaneacetic acid, 6,6-dimethyl-	U.S.	2,427,343	1947
		2,427,344	1947
Nystatin	Great Britain	714,189	1954
Paris green	France	809,586	1937
		811,622	1937
		49,607	1939*
	Germany	659,301	1938
		714,412	1941
		725,942	1942
		739,627	1943
2,4-Pentanedione	U.S.	2,158,071	1939

(continued)

*Reissue

Compound	Country	Patent Number	Year
2,4-Pentanedione (concluded)	U.S.	2,369,250	1945
		2,395,012	1946
		2,395,800	1946
Phenanthrenequinone	U.S.	2,401,028	1946
	Great Britain	508,526	1939
Phenol, o-chloro-	U.S.	2,603,662	1952
Phenol, o-(chloromercuri)-	U.S.	1,787,581	1931
		2,502,382	1950
	Canada	381,287	1939
Phenol, p-(chloromercuri)-	U.S.	1,787,581	1931
		2,502,382	1950
Phenol, 2,4-dichloro-	U.S.	2,440,602	1948
	Germany	349,794	1923
	Great Britain	573,475	1945
	Japan	3,896	1950
Phenol, 2,4-dinitro-	U.S.	1,320,076	1919
		2,455,322	1948
	Great Britain	131,403	1918
		140,955	1919
Phenol, 2,2'-methylenebis(4-chloro-	U.S.	2,334,408	1943
		2,662,040	1953
Phenol, o-nitro-	U.S.	2,577,041	1951
Phenol, pentachloro-	U.S.	2,107,650	1938
		2,131,259	1938
		2,176,417	1939
		2,304,013	1942
		2,548,646	1951
		2,563,815	1951
		2,576,987	1951
		2,577,041	1951
		2,608,591	1952
		2,644,015	1953
		2,662,918	1953
		2,692,899	1954
		2,708,640	1955
	Belgium	487,244	1949
		495,513	1950
	France	930,814	1948
		985,530	1951
	Great Britain	716,995	1954
		718,779	1954
	Italy	436,820	1948
	Japan	2,714	1951
		4,937	1951
		3,229	1952
		3,669	1953
		4,950	1954
Phenol, pentachloro-, sodium derivative	U.S.	2,483,008	1949
		2,637,661	1953

Compound	Country	Patent Number	Year
Phenol, pentachloro-, sodium derivative (concluded)	Great Britain	718,779	1954
	Italy	488,305	1953
Phenol, o-phenyl	U.S.	2,461,963	1949
		2,469,914	1949
	Japan	134,221	1940
Phenol, o-phenyl-, sodium derivative	US	2,386,954	1945
		2,469,914	1949
		2,489,744	1949
Phenol, 2,3,4,6-tetrachloro-	U.S.	2,304,013	1942
Phenol, 2,4,5-trichloro-	U.S.	2,304,013	1942
		2,509,245	1950
		2,577,041	1951
		2,665,314	1954
	Germany	349,794	
	Great Britain	672,499	1952
	Japan	2,672	1951
Phenol, 2,4,6-trichloro-	U.S.	2,304,013	1942
Phenothiazine	U.S.	2,284,124	1942
		2,294,888	1943
		2,295,074	1943
		2,353,292	1944
		2,360,295	1944
		2,402,686	1946
Potassium iodide	U.S.	2,278,053	1942
		2,415,346	1947
		2,715,582	1955
	U.S.S.R.	54,410	1939
2-Propen-1-ol, 2-methyl-, carbanilate	U.S.	2,370,578	1945
8-Quinolinol	U.S.	2,489,530	1949
		2,524,738	1950
		2,561,553	1951
		2,678,314	1954
	France	977,687	1951
	Great Britain	659,890	1951
8-Quinolinol, 5-chloro-7-iodo-	Germany	697,731	1940
	India	34,380	1948
8-Quinolinol, copper (II) derivative	U.S.	2,381,863	1945
		2,457,025	1948
		2,561,553	1951
		2,632,746	1953
		2,678,314	1954
		2,698,263	1954
	Great Britain	659,890	1951
	Holland	71,829	1953
Resorcinol, 4-hexyl-	Japan	2,671	1951

Compound	Country	Patent Number	Year
Safrole	Japan	2,247	1951
Salicylanilide	U.S.	2,576,987	1951
		2,578,752	1951
		2,691,010	1954
	Germany	808,991	1951
	Great Britain	7,875	1913
		408,258	1934
	Holland	59,151	1947
Salicylic acid	U.S.	1,265,378	1918
		1,380,277	1921
		2,524,738	1950
		2,576,987	1951
		2,595,181	1952
	France	458,724	1913
	Germany	901,175	1954
	Great Britain	103,739	1916
		105,613	1916
	Switzerland	78,108	1918
Salicylic acid, 3-phenyl-, copper II salt	U.S.	2,480,084	1949
Salol	U.S.	2,141,985	1938
	U.S.S.R.	37,098	1934
Semicarbazide, 3-thio-	U.S.	2,450,406	1948
		2,646,447	1953
		2,657,234	1953
	Germany	832,891	1952
	Great Britain	684,647	1952
	Japan	1,871	1952
		3,967	1952
		4,159	1952
	Sweden	130,297	1950
Sodium azide	U.S.	2,373,800	1945
	Japan	3,475	1954
Sodium chromate	U.S.	2,077,096	1937
		2,176,685	1939
		2,494,215	1950
	Austria	126,700	1948
	Great Britain	18,434	1908
		197,223	1922
		558,083	1943
	Italy	441,008	1948
		456,120	1950
	Japan	172,474	1946
Sodium fluoride	U.S.	1,324,030	1919
		1,382,165	1921
		1,464,990	1923
		2,058,075	1936
		2,585,387	1952
		2,690,430	1954
		2,692,186	1954

Compound	Country	Patent Number	Year
Sodium fluoride (concluded)	Canada	191,467	1919
	France	483,619	1917
		809,718	1937
	Germany	253,284	1910
		284,043	1912
		643,286	1937
	Great Britain	103,118	1916
		226,491	1923
		479,362	1938
		547,924	1942
		554,126	1943
		647,395	1950
	Italy	488,305	1953
	U.S.S.R.	36,393	1934
		43,415	1935
		52,709	1938
		53,142	1938
		54,030	1938
Sorbic acid	U.S.	2,484,067	1949
4,4'-Stilbenedicarboxamidine	U.S.	2,204,983	1940
		2,364,200	1944
	Great Britain	510,097	1939
4,4'-Stilbenedicarboxamidine, diisethionate	U.S.	2,394,003	1946
	Great Britain	559,015	1944
		575,145	1946
4,4'-Stilbenediol, α,α'diethyl-	U.S.	2,311,093	1943
		2,392,852	1946
		2,402,054	1946
	Germany	715,542	1941
		804,102	1951
	Great Britain	526,927	1940
		574,899	1946
		596,095	1947
		668,494	1952
	Hungary	123,817	1940
		124,314	1940
		135,060	1948
	Sweden	115,816	1946
Sulfanilamide, N^1-(2,6-dimethyl-4-pyrimidinyl)-	U.S.	2,351,333	1944
		2,386,852	1945
		2,429,184	1947
		2,482,085	1949
	Austria	175,895	1953
	Great Britain	553,205	1943
		560,345	1944
		565,501	1944
		566,788	1945
		582,149	1946
		589,040	1947

(continued)

Compound	Country	Patent Number	Year
Sulfanilamide, N^1-(2,6-dimethyl-4-pyrimidinyl)- (concluded)	India	39,684	1949
	Switzerland	220,347	1942
		230,865	1944
		231,194	1944
		242,053	1946
Sulfathiazole	U.S.	2,339,083	1944
		2,386,852	1945
		2,592,859	1952
	Australia	112,885	1941
	Austria	172,609	1952
	Denmark	67,896	1948
	France	848,175	1939
		972,920	1951
	Great Britain	566,788	1945
	Hungary	138,815	1948
		135,587	1949
	Japan	175,578	1948
		177,091	1948
		177,625	1948
		180,618	1949
		2,836	1950
		4,205	1950
		2,414	1951
		4,624	1953
	Spain	197,070	1952
	Switzerland	210,425	1940
		222,732	1942
		229,079	1944
		229,080	1944
		229,081	1944
		229,082	1944
		229,743	1944
Sulfide, bis(dimethylthiocarbamyl)-	U.S.	1,788,632	1931
		2,099,773	1937
		2,453,460	1948
		2,524,081	1950
		2,524,738	1950
		2,706,205	1955
	France	789,500	1935
	Great Britain	437,653	1935
	Italy	438,135	1948
2-Thiazolethiol, 4,5-dimethyl-	U.S.	2,603,646	1952
	Germany	678,153	1939
Thymol	U.S.	1,306,512	1919
		1,332,680	1920
		1,378,939	1921
		1,412,937	1922

Compound	Country	Patent Number	Year
Thymol (concluded)	U.S.	1,432,298	1923
		1,449,121	1923
		2,286,953	1942
		2,419,093	1947
		2,468,670	1949
		2,476,555	1949
	Great Britain	186,202	1921
		197,848	1922
		200,151	1922
		214,866	1923
		220,953	1923
		221,226	1923
		221,227	1923
		551,624	1943
		571,137	1945
	Japan	133,334	
	Switzerland	185,671	1937
Trichomycin	Japan	4,200	1954
Triethylene glycol	U.S.	2,654,786	1953
	Japan	156,570	1943
		178,420	1949
Uracil, 2-thio-	Japan	849	1950
		850	1950
Urea, thio-	U.S.	2,173,067	1939
		2,266,221	1942
		2,337,882	1943
		2,353,997	1944
		2,357,149	1944
		2,393,917	1946
		2,417,318	1947
		2,521,778	1950
		2,552,584	1951
		2,560,596	1951
	Germany	260,061	1911
		266,404	1912
		717,094	1942
	Great Britain	634,463	1950
		645,701	1950
		645,702	1950
	Japan	2,876	1950
		285	1951
		1,149	1951
		7,218	1951
		5,129	1952
Vitamin B_6 hydrochloride	U.S.	2,349,267	1944

(continued)

Compound	Country	Patent Number	Year
Vitamin B_6 hydrochloride (concluded)	U.S.	2,410,531	1946
		2,410,938	1946
		2,422,195	1947
		2,442,677	1948
		2,483,137	1949
	Great Britain	567,611	1945
		625,997	1949
		629,450	1949
	Japan	161,769	1944
		2,141	1952

APPENDIX II. ADDITIONAL COMPOUNDS HAVING FUNGICIDAL PROPERTIES

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Acrylic acid, 2-chloro-3-hydroxy-, benzoate, ethyl ester [55]
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