

5. TABLES

TABLE 5.1
 VON BAEYER/IUPAC NAMES OF DIELDRIN (HEOD) AND RELATED COMPOUNDS

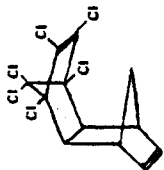
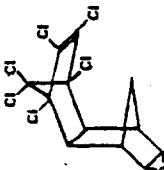
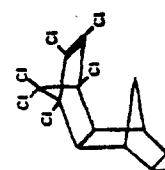
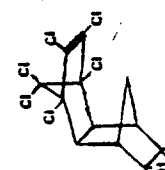
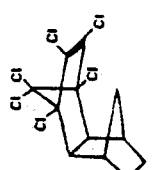
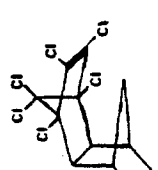
Abbreviated Chemical Names and Other Designations	Von Bayer/IUPAC Name	CAS No.*	Molecular Weight	Molecular Formula	Structure
Aldrin HHDN SD 2794	1,8,9,10,11,11-Hexachloro-2,3-7,6-endo-2,1-7,8-exo-tetracyclo-(6.2.1.1.1,3,6,0,2,7)dodeca-4,9-ene	309-00-2	364.9	C ₁₂ H ₈ Cl ₆	
Dieldrin HEOD SD 3417	1,8,9,10,11,11-Hexachloro-4,5-exo-epoxy-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.1,3,6,0,2,7)dodec-9-ene	60-57-1	380.9	C ₁₂ H ₈ Cl ₆ O	
cis-4,5-Dihydroxy-dihydroaldrin "Aldrin cis-diol" WL 43020	1,8,9,10,11,11-Hexachloro-4,5-(exo)cis-dihydroxy-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.1,3,6,0,2,7)dodec-9-ene	30460-74-3	398.9	C ₁₂ H ₁₀ Cl ₆ O ₂	
trans-4,5-Dihydroxy-dihydroaldrin "trans-6,7-Dihydroxy-dihydroaldrin" "Aldrin trans-diol" WL 40549	1,8,9,10,11,11-Hexachloro-4,5-trans-dihydroxy-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.1,3,6,0,2,7)dodec-9-ene	3106-29-4	398.9	C ₁₂ H ₁₀ Cl ₆ O ₂	
4,5-Dihydroaldrin	1,8,9,10,11,11-Hexachloro-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.1,3,6,0,2,7)dodec-9-ene	10059-65-1	366.9	C ₁₂ H ₁₀ Cl ₆	
4-Ketodihydroaldrin	1,8,9,10,11,11-Hexachloro-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.1,3,6,0,2,7)dodec-9-ene-4-one	34022-77-0	380.9	C ₁₂ H ₈ Cl ₆ O	

TABLE 5.1 (continued)
 VON BAEYER/IUPAC NAMES OF DIELDRIN (HEOD) AND RELATED COMPOUNDS

Abbreviated Chemical Names and Other Designations	Von Baeyer/IUPAC Name	CAS No.*	Molecular Weight	Molecular Formula	Structure
Photodieldrin "Photoisomer of dieldrin" "Photo-HEOD" BI 6623	3,exo-4,5,6,6,7-Hexachloro-11,12-exo-epoxy-pentacyclo-(6.4.0.0.2 ¹⁰ .3 ⁷ .05,9)dodecane INCORRECT NAME: 1,9,10,10,11-exo-12-Hexachloro-4,5-exo-epoxy-8,3-7,6-endo-8,9-7,11-exo-pentacyclo-(7.3.0.0.2 ⁶ .03 ⁸ .07,11)dodecane	13366-73-9	380.9	C ₁₂ H ₈ Cl ₆ O	
4-Keto-4-dechloro-photodieldrin "HEOD Pentachloroketone" "Ketophotodieldrin" "Klein's metabolite"	3,5,6,6,7-Pentachloro-11,12-exo-epoxy-pentacyclo-(6.4.0.0.2 ¹⁰ .3 ⁷ .05,9)dodecan-4-one INCORRECT NAME: 1,9,10,10,11-Pentachloro-4,5-exo-epoxy-8,9-7,11-exo-pentacyclo-(7.3.0.0.2 ⁶ .03 ⁸ .07,11)dodecan-1,2-one	21039-31-3	360.5	C ₁₂ H ₇ Cl ₅ O ₂	
4,5-seco-Aldrin-4,5-dicarboxylic acid (seco-ADA) "Aldrin dicarboxylic acid" "Dihydrochlordene dicarboxylic acid" "Aldrin-derived acid" "ADA" SD 2878	1,7,8,9,10,10-Hexachloro-2,3-6,5-endo-tricyclo(5.2.1.0 ^{2,6} .04,8)dec-8-ene-3,5-exo,exo-dicarboxylic acid	5103-66-2	428.9	C ₁₂ H ₈ Cl ₆ O ₄	
11,12-seco-Photoaldrin-11,12-dicarboxylic acid "Acid from oxidation of photoaldrin"	1,7,8,exo-9,10,10-Hexachlorotetracyclo(5.2.1.0 ^{2,6} .04,8)decane-3,5-exo,exo-dicarboxylic acid	428.9	428.9	C ₁₂ H ₈ Cl ₆ O ₄	

Adapted from Bedford 1974

TABLE 5.1 (continued)

VON RAEYER/IUPAC NAMES OF DIELDRIN (HEOD) AND RELATED COMPOUNDS

Abbreviated Chemical Names and Other Designations	Von Raeyer/IUPAC Name	CAS No.*	Molecular Weight	Molecular Formula	Structure
syn-12-Hydroxy-dieldrin "9-Hydroxy HEOD" WL 40231	1,8,9,10,11,11-hexachloro-4,5-exo-epoxy-12-(syn-epoxy)hydroxy-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.3,6.02,7)dodec-9-ene	26946-01-0	396.9	$C_{12}H_8Cl_6O_2$	
12-Ketodieldrin "9-Keto-HEOD" WL 42170	1,8,9,10,11,11-Hexachloro-4,5-exo-epoxy-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.3,6.02,7)dodec-9-en-12-one		394.9	$C_{12}H_6Cl_6O_2$	
9-Dechloroaldrin "Pentachloro photoproduct of aldrin"	1,8,10,11,11-Pentachloro-2,3-7,6-endo-2,1-7,8-exo-tetracyclo(6.2.1.1.3,6.02,7)dodeca-4,9-diene	21939-95-6	330.5	$C_{12}H_9Cl_5$	
9-Dechlorodieldrin "Pentachloro photoproduct of HEOD" "pentachlorodieldrin"	1,8,10,11,11-pentachloro-4,5-exo-epoxy-2,3-7,6-endo-2,1-7,6-exo-tetracyclo(6.2.1.1.3,6.02,7)dodec-9-ene		362.5	$C_{12}H_9Cl_5O$	
Photoaldrin "Photoisomer of aldrin" SD 18303	3,exo-4,5,6,6,7-hexachloropentacyclo(6.4.0.0.2,10.03,7.05,9)dodec-11-ene	13366-64-8	364.9	$C_{12}H_8Cl_6$	

TABLE 5.2

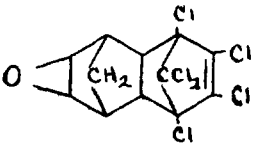
PHYSICAL AND CHEMICAL PROPERTIES OF ALDRIN

Appearance	Brown to white crystalline solid
Empirical formula	$C_{12}H_8Cl_6$
Structure	
Molecular weight	364.93
Melting point	104-105.5 C
Vapor pressure	2.31×10^{-5} mm Hg at 20 C
Octanol/water partition coefficient	5.00
Solubility	Insoluble in water; very soluble in most organic solvents
Stability	Stable in the presence of organic and inorganic alkalis; stable to the action of hydrated metal chlorides

From IARC 1974, Condensed Chemical Dictionary 1977, Merck 1976

TABLE 5.3

PHYSICAL AND CHEMICAL PROPERTIES OF DIELDRIN

Appearance	Light tan, flaked solid
Empirical formula	$C_{12}H_8OCl_6$
Structure	
Molecular weight	380.93
Melting point	175 C
Vapor pressure	1.78×10^{-7} mm Hg at 20 C
Octanol/water partition coefficient	4.56
Solubility	Practically insoluble in water (0.25 mg/liter); moderately soluble in common organic solvents except aliphatic petroleum solvents and methyl alcohol
Stability	Stable in organic and inorganic alkalis and acids commonly used in agriculture

From IARC 1974, Condensed Chemical Dictionary 1977, Merck 1976

TABLE 5.4

SYNONYMS AND TRADE NAMES FOR ALDRIN AND DIELDRIN

Aldrin

1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene

Compound 118

Octalene

HHDN

SD 2794

Dieldrin

3,4,5,6,9,9-Hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene

1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-endo,exo-1,4:5,8-dimethanonaphthalene

Compound 497

Insecticide No. 497

HEOD

Octalox

SD 3417

From Condensed Chemical Dictionary 1977, Merck 1976

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