4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

The naturally-occurring pyrethrins, extracted from chrysanthemum flowers, are esters of chrysanthemic acid (Pyrethrin I, Cinerin I, and Jasmolin I) and esters of pyrethric acid (Pyrethrin II, Cinerin II, and Jasmolin II). In the United States, the pyrethrum extract is standardized as 45–55% w/w total pyrethrins. The typical proportion of Pyrethrins I to II is 0.2:2.8, while the ratio of pyrethrins:cinerins:jasmolins is 71:21:7 (Tomlin 1997). Information regarding the chemical identity of the pyrethrins is presented in Table 4-1.

Pyrethroids are synthetic esters derived from the naturally-occurring pyrethrins. One exception to the axiom that all pyrethroids are esters of carboxylic acids is noteworthy. There is a group of oxime ethers that exhibits insecticidal activity similar in nature to the pyrethrins and pyrethroid esters (Davies 1985). Little data exist regarding these compounds, and no commercial products have been produced. Commercially available pyrethroids include allethrin, bifenthrin, bioresmethrin, cyfluthrin, cyhalothrin, cypermethrin, deltamethrin, esfenvalerate (fenvalerate), flucythrinate, flumethrin, fluvalinate, fenpropathrin, permethrin, phenothrin, resmethrin, tefluthrin, tetramethrin, and tralomethrin. Information regarding the chemical identity of pyrethroids is shown in Table 4-2.

With the exception of deltamethrin, pyrethroids are a complex mixture of isomers rather than one single pure compound. For pyrethroids possessing the cyclopropane moiety, isomerism about the cyclopropane ring greatly influences the toxicity of these insecticides. The presence of two chiral centers in the ring results in two pairs of diastereomers. The diastereomers and their nonsuperimposable mirror images (enantiomers) are illustrated in Figure 4-1. In this figure, the C-1 position of the ring is assigned to the carbon atom bonded to the ester moiety. It is also customary to designate the stereochemistry at the C-3 position as simply cis or trans relative to the ester group bonded to C-1 rather than assigning its absolute configuration. The 1R conformations about the cyclopropane ring are considerably more toxic than the 1S isomers. Both the cis and trans isomers show insecticidal activity, but have differing mammalian toxicities, with the cis isomers being more potent (Ray 1991). Pyrethroids that contain a cyano substituent at the alcohol moiety (Type II pyrethroids) demonstrate differing toxicity based upon the optical isomerism of the alpha carbon. It has been demonstrated that the S conformation about the alpha carbon is considerably more toxic towards insects when compared to the R conformation (Dorman and

Table 4-1. Chemical Identity of the Pyrethrins

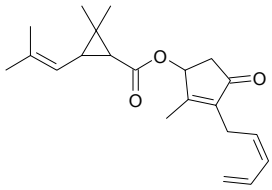
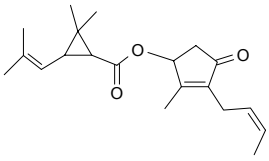
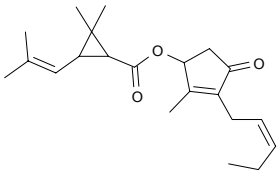
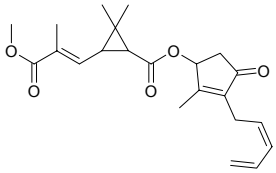
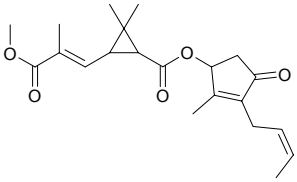
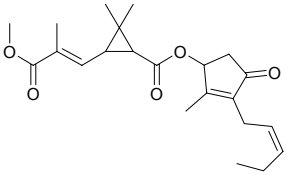
Characteristic	Pyrethrin I	Cinerin I	Jasmolin I
Synonym(s)[b]	(Z)-(S)-2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclo pent-2-enyl (1R)-trans-2,2-dimethyl-3-(2-methyl prop-1-enyl)cyclo-propanecarboxylate	(Z)-(S)-3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl (1R)-trans-2,2-di methyl-3-(2-methyl prop-1-enyl)cyclo-propanecarboxylate	(Z)-(S)-2-methyl-4-oxo-3-(pent-2-enyl)cyclopent-2-enyl (1R)-trans-2,2-di-methyl-3-(2-methylprop-1-enyl)-cyclopro-panecarboxylate
Ratio of isomers	Pure isomer	Pure isomer	Pure isomer
Registered trade name(s)	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl
Chemical formula	$C_{21}H_{28}O_3$	$C_{20}H_{28}O_3$	$C_{21}H_{30}O_3$
Chemical structure			
Identification numbers:			
CAS registry	121-21-1	25402-06-6	4466-14-2
NIOSH RTECS[c]	GZ1725000	GZ1540000	No data
EPA hazardous wasted	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	6302
HSDB[d]	6302	6837	No data
NCI	No data	No data	No data

Table 4-1. Chemical Identity of the Pyrethrins

Characteristic	Pyrethrin II	Cinerin II	Jasmolin II
Synonym(s)[b]	(Z)-(S)-2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclo pent-2-enyl (E)-(1R)-trans-3-(2-methoxy carbon ylprop-1-enyl)-2,2-dimethylcyclopropane-carboxylate	(Z)-(S)-3-(but-2-enyl)-2-methyl-4-oxocyclopent-2-enyl (E)-(1R)-trans-3-(2-methoxycarbonylprop-1-enyl)-2,2-dimethyl cyclopropanecarboxylate	(Z)-(S)-2-methyl-4-oxo-3-(pent-2-enyl)cyclopent-2-enyl (E)-(1R)-trans-3-(2-methoxycarbonylprop-1-enyl)-2,2-dimethylcyclo-propanecarboxylate
Ratio of isomers	Pure isomer	Pure isomer	Pure isomer
Registered trade name(s)	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl	Alfadex, Evergreen, ExciteR, Milon, Pycon, Pyrocide, Pyronyl
Chemical formula	$C_{22}H_{28}O_5$	$C_{21}H_{28}O_5$	$C_{22}H_{30}O_3$
Chemical structure			
Identification numbers:			
CAS registry	121-29-9	121-20-0	1172-63-0
NIOSH RTECS[c]	GZ0700000	No data	No data
EPA hazardous wasted	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	6303	6838	No data
NCI	No data	No data	No data

[a]All information obtained from Tomlin, 1997 except where noted.
[b]Chemical names used are those currently indexed by the Chemical Abstracts Service.
[c]NIOSH 1987
[d]HSDB 2001
[e] WHO 2001

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS =Registry of Toxic Effects of Chemical Substances

Table 4-2. Chemical Identity of Selected Pyrethroids[a]

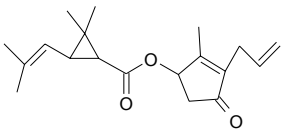
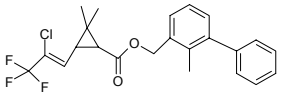
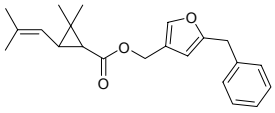
Characteristic	Allethrin	Bifenthrin	Bioresmethrin
Synonym(s)[b]	2-methyl-4-oxo-3-(2-propenyl)-2-cyclopenten-1-yl 2,2-dimethyl-3-(2-methyl-1-propenyl)cycloprane-carboxylate	(2-methyl[1,1'-biphenyl]-3-yl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropane-carboxylate	(1R-trans)-[5-phenylmethyl)-3-furanyl]mehtyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropane-carboxylate
Ratio of isomers	≥95% (1R)-isomers ≥75% trans-isomers	≥97% cis-isomer	≥90% (1R)-trans-isomer
Registered trade name(s)	Pyresin, Pynamin Forte, Exthrin	Talstar	Isathrine
Chemical formula	$C_{19}H_{26}O_3$	$C_{23}H_{22}ClF_3O_2$	$C_{22}H_{26}O_3$
Chemical structure			
Identification numbers:			
CAS registry	584-79-2	82657-04-3	28434-01-7
NIOSH RTECS[c]	GZ1925000	GZ1227800	GZ1227800
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	NA2902, NA2588, UN2588, UN2902, UN2903, UN3201, IMO3.2, IMO6.1	No data	No data
HSDB[d]	1511	6568	6568
NCI	No data	No data	No data

Table 4-2. Chemical Identity of Selected Pyrethroids[a]

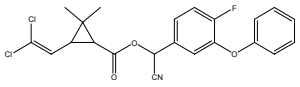
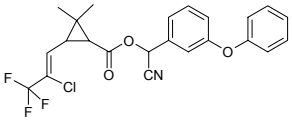
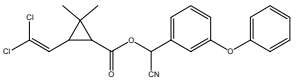
Characteristic	Cyfluthrin	Cyhalothrin	Cypermethrin
Synonym(s)[b]	Cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate	[1α,3α(Z)]-(±)-Cyano-(3-phenoxyphenyl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)2,2-dimethylcyclopropanecarboxylate	Cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloro ethenyl)-2,2-dimethyl-cyclopropanecarboxylate
Ratio of isomers	Unstated stereochemistry	≥95% cis-isomers	Unstated stereochemistry
Registered trade name(s)	Baythroid, Baygon aerosol, Solfac[b]	Cyhalon, Grenade	Arrivo, Cymbush, Cymperator, Cynoff, Ripcord, Basathrin, Demar, Grand, Starcyp[b]
Chemical formula	$C_{22}H_{18}Cl_2FNO_3$	$C_{23}H_{19}ClF_3NO_3$	$C_{22}H_{19}Br_2NO_3$
Chemical structure			
Identification numbers:			
CAS registry	68359-37-5	68085-85-8	52315-07-8
NIOSH RTECS[c]	GZ1253000	GZ122770	GZ1250000
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	6599	6791	6600
NCI	No data	No data	No data

Table 4-2. Chemical Identity of Selected Pyrethroids[a]

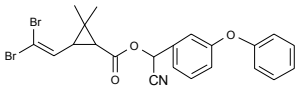
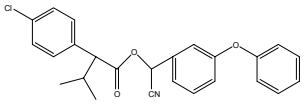
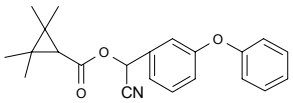
Characteristic	Deltamethrin	Esfenvalerate	Fenpropathrin
Synonym(s)[b]	[1R-[1α(S*),3α]]-Cyano (3-phenoxy-phenyl)methyl 3-(2,2-dibromo ethenyl)-2,2-dimethylcyclopropane-carboxylate, decamethrin	{S-R*,R*]-Cyano(3-phenoxyphenyl)methyl 4-chloro-2-(1-methyl-ethyl)benzeneacetate, fenvalerate	Cyano(3-phenoxy-phenyl)methyl 2,2,3,3-tetramethyl-cyclopropane-carboxylate(racemate) fenpropanate (unspecified)
Ratio of isomers	≥98% single isomer	≥75% (S,S)-isomers	Unstated stereochemistry
Registered trade name(s)	Butox, Decis, K-Othrin, Kordon, Sadethrin[b]	Sumi-alfa, Sumi-alpha, Asana (esfenvalerate), Pydrin, Ectrin,Sumicidin, Arfen, Dufen, Fenval (fenvalerate)[b]	Danitol, Herald, Meothrin, Rody, Digital[b]
Chemical formula	$C_{22}H_{19}Br_2NO_3$	$C_{25}H_{22}ClNO_3$	$C_{22}H_{23}NO_3$
Chemical structure			
Identification numbers:			
CAS registry	52918-63-5	66230-04-4, 51630-58-1 (fenvalerate)	64257-84-7 (racemic), 39515-41-8 (stereochemistry)
NIOSH RTECS[c]	GZ1233000, GZ1232000	CY1576367, CY1576350	GZ2090500, GZ2090000
EPA hazardous waste	No data	CY1576350	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	6604	6625, 6640	6636
NCI	No data	No data	No data

Table 4-2. Chemical Identity of Selected Pyrethroids[a]

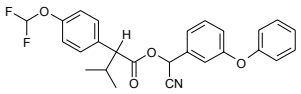
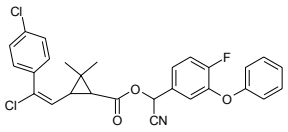
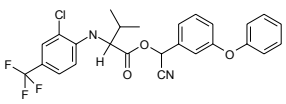
Characteristic	Flucythrinate	Flumethrin	Fluvalinate
Synonym(s) [b]	Cyano(3-phenoxy-phenyl)methyl 4-(difluoromethoxy)-α-(1-methylethyl)benzene-acetate	α-Cyano-4-fluoro-3-phenoxybenzyl 3-(ß,4-dichlorostyryl)-2,2-dimethylcyclopropane-carboxylate	Cyano(3-phenoxy-phenyl)methyl N-N-[2-chloro-4-(trifluoro-methyphenyl)-DL-valinate, D-valinate
Ratio of isomers	No data	Unstated stereochemistry	Tau-fluvalinate is a 1:1 mixture of (R)-a-cyano, 2-(R) and (S)-a- cyano, 2-(R) diasteriomers
Registered trade name(s)	Cybolt, Cythrin, Pay-off, Fluent	Bayticol, Bayvarol	Klartan, Mavrik
Chemical formula	$C_{26}H_{23}F_2NO_4$	$C_{28}H_{22}Cl_2FNO_3$	$C_{26}H_{22}ClF_3N_2O_3$
Chemical structure			
Identification numbers:			
CAS registry	70124-77-5	69770-45-2	69409-94-5, 102851-06-9 (tau-fluvalinate)
NIOSH RTECS[c]	CY1578620	No data	YV9397100
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	6647	No data	6659
NCI	No data	No data	No data

Table 4-2. Chemical Identity of Selected Pyrethroids[a]

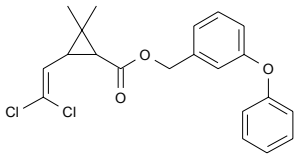
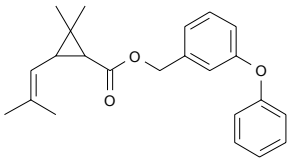
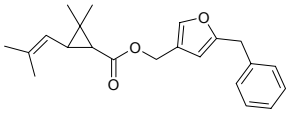
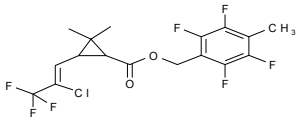
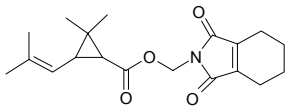
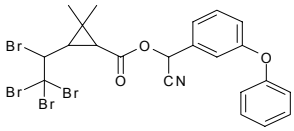
Characteristic	Permethrin	Phenothrin	Resmethrin
Synonym(s)[b]	(3-Phenoxyphenyl)methyl3-(2,2-dichloroehenyl)-2,2-dimethylcyclopropane-carboxylate	(3-Phenoxyphenyl)methyl-2,2-dimethyl-3-(2-methyl-1-propenyl)-cyclopropanecarboxylate	[5-Phenylmethyl)-3-furanyl]mehtyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropane-carboxylate
Ratio of isomers	(1R, trans):(1R,cis):(1S, trans):(1S, cis)=3:2:3:2[e]	Mixed isomers	20–30% (1RS)-cis-isomers 80–70% (1(RS)-trans-isomers)
Registered trade name(s)	Ambush, Assithrin, Cliper, Coopex, Corsair, Dragnet, Dragon, Kafil, Eksmin, Perkill, Pounce	Sumithrin	Synthrin, Chrysron
Chemical formula	$C_{21}H_{20}Cl_2O_3$	$C_{23}H_{26}O_3$	$C_{22}H_{26}O_3$
Chemical structure			
Identification numbers:			
CAS registry	52645-53-1	26002-80-2	10453-86-8
NIOSH RTECS[c]	GZ1255000	GZ1975000	GZ1310000
EPA hazardous wasted	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	6740	3922	6790
NCI	No data	No data	No data

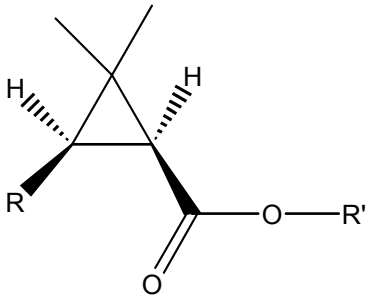
Table 4-2. Chemical Identity of Selected Pyrethroids[a]

Characteristic	Tefluthrin	Tetramethrin	Tralomethrin
Synonym(s) [b]	[1α,3α(Z)]-(±)-(2,3,5,6-Tetrafluoro-4-methylphenyl)methyl 3-(2-chloro-3,3,3-trifluoro-1propenyl)-2,2-dimethyl-cyclopropanecarboxylate	(1,3,4,5,6,7-Hexahydro-1,3-dioxo-2H-isoindol-2-yl)methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)-cyclopropanecarboxylate	Cyano(3-phenoxyphenyl)-methyl 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)-cyclopropanecarboxylate
Ratio of isomers	Mixture of isomers	(1R, trans):(1R,cis):(1S, trans):(1S, cis)=4:1:4:1[e]	Unstated stereochemistry
Registered trade name(s)	Force, Fireban	Neo-Pynamin, Duracide	Saga, Scout, Tralox, Tracker, Tralate
Chemical formula	$C_{17}H_{14}ClF_7O_2$	$C_{19}H_{25}NO_4$	$C_{22}H_{19}Br_4NO_3$
Chemical structure			
Identification numbers:			
CAS registry	79538-32-2	7696-12-0	66841-25-6
NIOSH RTECS[c]	GZ1227850	GX1730000	GZ2009500
EPA hazardous waste	No data	No data	No data
OHM/TADS	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data
HSDB[d]	No data	6738	6604
NCI	No data	No data	No data

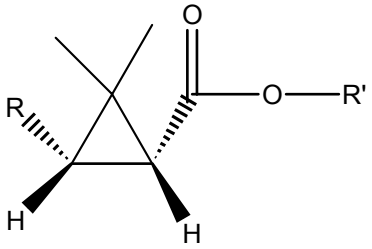
[a]All information obtained from Tomlin, 1997 except where noted.
[b]Chemical names used are those currently indexed by the Chemical Abstracts Service.
[c]NIOSH 1987
[d]HSDB 2001
[e] WHO 2001

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS =Registry of Toxic Effects of Chemical Substances

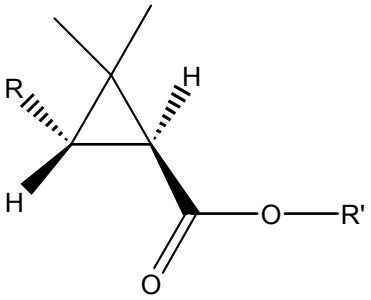
Figure 4-1. Four Possible Isomers of Type I Pyrethroids



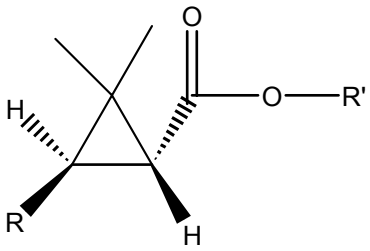
1S *cis* configuration



1R *cis* configuration



1S *trans* configuration



1R *trans* configuration

Beasley 1991). Figure 4-2 illustrates the S conformation of the type II pyrethroid cyhalothrin about the alpha carbon. Pyrethroids such as cyfluthrin, cypermethrin, and cyhalothrin possess three chiral centers, and thus consist of eight possible isomers. The production of pyrethroids with differing isomeric ratios is one reason for the wide variation in reported toxicities of these compounds. For example, cypermethrin is formulated as four different insecticides (alpha-, beta-, theta- and zeta-cypermethrin) depending upon the ratio of the different isomers; and each of these products has different toxicologic properties. The complex compositions of several important pyrethroids are illustrated in Table 4-3.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of the pyrethrins and selected pyrethroids are located in Tables 4-4 and 4-5, respectively. Generally, pyrethrins and pyrethroids have low vapor pressures, low Henry's law constants, and large octanol/water coefficients (K_{ow}), and are not very soluble in water. Aside from their interaction with polarized light, enantiomers possess identical physical properties (e.g., boiling point, melting point, solubility, etc.). Diastereomers have different physical properties however, and changes in the geometrical isomeric composition can lead to different values in the properties reported for the pyrethroids listed in Table 4-5.

Table 4-3. Stereoisomers of Selected Pyrethroids[a]

Pyrethroid	Different products	Isomer composition
Cypermethrin	alpha-cypermethrin	Racemic mixture comprised of: (S)-alpha-cyano-3-phenoxybenzyl-(1R)-cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (R)-alpha-cyano-3-phenoxybenzyl-(1S)-cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate
	beta-cypermethrin	Mixture comprised of two enantiomeric pairs in a 2:3 ratio: (S)-alpha-cyano-3-phenoxybenzyl-(1R)-cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (R)-alpha-cyano-3-phenoxybenzyl-(1S)-cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate with (S)-alpha-cyano-3-phenoxybenzyl-(1R)-trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate and (R)-alpha-cyano-3-phenoxybenzyl-(1S)-trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclo-propanecarboxylate
	theta-cypermethrin	Racemic mixture comprised of: (S)-alpha-cyano-3-phenoxybenzyl-(1R)-trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (R)-alpha-cyano-3-phenoxybenzyl-(1S)-trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate
	zeta-cypermethrin	Mixture of the stereoisomers: (S)-alpha-cyano-3-phenoxybenzyl(1RS,3RS;1RS,3SR)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate where the ratio of the (S); (1RS,3RS) isomeric pair to the (S);(1RS,3SR) isomeric pair lies in the range of 45-55 to 55-45.

Table 4-3. Stereoisomers of Selected Pyrethroids[a]

Pyrethroid	Different products	Isomer composition
Cyfluthrin	cyfluthrin	Comprised of a mixture of the 4 diastereomeric pairs of enantiomers: I = (R)-alpha-cyano-4-fluoro-3-phenoxybenzyl-(1R)-cis -3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate + (S)-alpha, (1S)-cis II = (S)-alpha-cyano-4-fluoro-3-phenoxybenzyl-(1R)-cis -3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate + (R)-alpha, (1S)-cis III = (R)-alpha-cyano-4-fluoro-3-phenoxybenzyl-(1R)-trans -3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate + (S)-alpha, (1S)-trans IV = (S)-alpha-cyano-4-fluoro-3-phenoxybenzyl-(1R)-trans -3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane-carboxylate + (R)-alpha, (1S)-trans The technical grade product consists of 23-26% I, 16-19% II, 33-36% III and 22-25% IV.
	beta-cyfluthrin	Mixture of II and IV in a 1:2 ratio.
Cyhalothrin	cyhalothrin	(RS)-alpha-cyano-3-phenoxybenzyl (Z) (1RS)-cis-3-(2-chloro-3,3,3-trifluoropropenyl)-2,2-dimethylcyclo-propanecarboxylate
	lambda-cyhalothrin	Racemic mixture comprised of: (S)-alpha-cyano-3-phenoxybenzyl (Z) (1R)-cis-3-(2-chloro-3,3,3-trifluoropropenyl)-2,2-dimethylcyclo-propanecarboxylate and (R)-alpha-cyano-3-phenoxybenzyl (Z) (1S)-cis-3-(2-chloro-3,3,3-trifluoropropenyl)-2,2-dimethylcyclopropane-carboxylate

[a]All information obtained from Tomlin 1997.

Table 4-4. Physical and Chemical Properties of Pyrethrins[a]

Property	Pyrethrin I	Cinerin I	Jasmolin I
Molecular weight	328.5	316.4	330.5
Color	No data	No data	No data
Physical state	Viscous liquid[b]	No data	No data
Melting point, °C	No data	No data	No data
Boiling point, °C	146–150 at 0.0005 mm Hg, 170 at 0.1 mm Hg[c]	136–138 at 0.008 mm Hg[d]	No data
Density, g/cm^3 at 25 °C	1.51 (18 °C)	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	0.2	Insoluble	0.03[i]
Organic solvent(s)	Soluble	Soluble	No data
Partition coefficients:			
Log K_{ow}	5.9	5.93[i]	6.42[i]
Vapor pressure, mm Hg at 25 °C	2.03x10^{-5}	1.1x10^{-6i}	4.8x10^{-7i}
Henry's Law constant, atm-m^3/mol at 25 °C	7.7x10^{-7i}	9.6x10^{-7i}	1.3x10^{-6i}
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	No data	No data	No data
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[e]	1 mg/m^3=0.074 ppm	1 mg/m^3=0.077 ppm	1 mg/m^3=0.074 ppm
Explosive limits	No data	No data	No data

Table 4-4. Physical and Chemical Properties of Pyrethrins[a]

Property	Pyrethrin II	Cinerin II	Jasmolin II
Molecular weight	372.5	360.4	357.7
Color	No data	No data	No data
Physical state	Viscous liquid[b]	Viscous oil[b]	No data
Melting point, °C	No data	No data	No data
Boiling point, °C	192–193 at 0.007 mm Hg, 200 at 0.1 mm Hg[c]	182–184 at 0.001 mm Hg	No data
Density, g/cm^3 at 25 °C	No data	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	9.0	Insoluble	0.09[i]
Organic solvent(s)	Soluble	Soluble	No data
Partition coefficients:			
Log K_{ow}	4.3	4.98[i]	5.47[i]
Vapor pressure, mm Hg at 25 °C	3.98x10^{-7}	4.6x10^{-7i}	1.9x10^{-7i}
Henry's Law constant, atm-m^3/mol at 25 °C	7.4x10^{-10i}	9.2x10^{-10i}	1.2x10^{-9i}
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	No data	No data	No data
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[e]	1 mg/m^3=0.066 ppm	1 mg/m^3=0.068 ppm	1 mg/m^3=0.065 ppm
Explosive limits	No data	No data	No data

[a]All information obtained from HSDB 2001 except where noted
[b]Technical grade
[c]Tomlin 1997
[d]Budavari 1996
[g]USDA 2001a
[e]These air conversion factors were calculated by using the average molecular weight and ideal gas law.
[f]Milne 1995
[h]Howard and Meylan 1997
[i]Estimated value from EPIWIN (Syracuse Research Corporation)

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids [a]

Property	Allethrin	Bifenthrin	Bioresmethrin[b]
Molecular weight	302.4	422.9	338.4
Color	Pale yellow[b,c]	Light brown[c]	Yellow to brown[c]
Physical state	Viscous liquid	Viscous oil	Viscous liquid[c]
Melting point, °C	~4	68–70	71.5-83[d]
Boiling point, °C	281.5	No data	Dec. >180
Density, g/cm^3 at 25 °C	1.01 (25 °C)	1.212 (25 °C)	1.050 (20 °C)
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	4.6 (25 °C)	0.1	<0.3 (25 °C)
Organic solvent(s)	Soluble	Soluble	Soluble
Partition coefficients:			
Log K_{ow}	4.8	6[e]	>4.7
Vapor pressure, mm Hg at 25 °C	1.2x10^{-6} (21 °C)	1.8x10^{-4d}	1.4x10^{-8}
Henry's Law constant, atm-m^3/mol at 25 °C	6.1x10^{-7i}	<1.0x10^{-3d}	1.3x10^{-7f}
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	87[b]	165[b]	92[b]
Flammability limits	No data	No data	No data
Conversion factors			
Air (25 °C1)[g]	1 mg/m^3=0.081 ppm	1 mg/m^3=0.058 ppm	1 mg/m^3=0.072 ppm
Explosive limits	No data	No data	No data

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids[a]

Property	Cyfluthrin	Cyhalothrin	Cypermethrin
Molecular weight[c]	453.3	449.9	416.3
Color	Yellowish brown[c]	Yellow-brown[c]	Yellow brown[b,c]
Physical state	Oil (A)	Viscous liquid[c]	Viscous semi-solid[b,c]
Melting point, °C	60 (A)	49.2[g]	80.5
Boiling point, °C	No data	187–190	No data
Density, g/cm^3 at 25 °C	No data	1.25	1.25
Odor	Aromatic	Mild	Odorless
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	0.002 (20 °C)[g]	0.003 (20 °C)	0.004 (20 °C)
Organic solvent(s)	Soluble	Soluble	Soluble
Partition coefficients:			
Log K_{ow}	5.94	6.9	6.6
Vapor pressure, mm Hg at 25 °C	2.03x10^{-9}[d]	1.5x10^{-9} (20 °C)[d]	3.07x10^{-9} (20 °C)
Henry's Law constant, atm-m^3/mol at 25 °C	9.5x10^{-7}[h]	1.8x10^{-7}[d]	4.2x10^{-7}[d]
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	107[b]	>100[b]	No data
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[e]	1 mg/m^3=0.054 ppm	1 mg/m^3=0.054 ppm	1 mg/m^3=0.059 ppm
Explosive limits	No data	No data	No data

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids[a]

Property	Deltamethrin	Esfenvalerate	Fenpropathrin
Molecular weight[c]	505.2	419.9	349.4
Color	Colorless	Colorless	Yellow brown[c]
Physical state	Crystals	Crystals	Solid[c]
Melting point, °C	101–102	59–60.2	45–50
Boiling point, °C	No data	151–167	No data
Density, g/cm^3 at 25 °C	0.55[b]	1.175	1.15 (25 °C)
Odor	Odorless	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	<0.002	0.0002 (25 °C)	0.014 (25 °C)[d]
Organic solvent(s)	Soluble	Soluble	Soluble
Partition coefficients:			
Log K_{ow}	6.1	4.0	6.0 (20 °C)
Vapor pressure, mm Hg at 25 °C	$1.5x10^{-8}$	$1.5x10^{-9}$	$5.5x10^{-6}$ (20 °C)
Henry's Law constant, atm-m^3/mol at 25 °C	$1.2x10^{-4}$	$4.1x10^{-7}$[d]	$1.8x10^{-4}$[g]
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	No data	256[b]	No data
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[g]	1 mg/m^3=0.048 ppm	1 mg/m^3=0.058 ppm	1 mg/m^3=0.070 ppm
Explosive limits	No data	No data	No data

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids[a]

Property	Flucythrinate	Flumethrin[b]	Fluvalinate
Molecular weight[c]	451.5	510.4	502.9
Color	Dark amber[b,c]	Yellowish[c]	Yellow-amber[c]
Physical state	Viscous liquid[c]	Viscous oil[c]	Viscous liquid[c]
Melting point, °C	No data	No data	No data
Boiling point, °C	108 at 0.35 mm Hg	>250	>450 164 at 0.07 mm Hg[b]
Density, g/cm^3 at 25 °C	1.189 (22 °C)	No data	1.29
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	0.5 (21 °C)	9.7×10^{-5}[f]	0.002
Organic solvent(s)	Soluble	No data	Soluble
Partition coefficients:			
Log K_{ow}	4.7[d]	7.65[i]	4.26[g]
Vapor pressure, mm Hg at 25 °C	8.5×10^{-9}[d]	3.9×10^{-9}[f]	5.7×10^{-7}[d]
Henry's Law constant, atm-m^3/mol at 25 °C	8.47×10^{-8}[d]	4.2×10^{-8}[f]	3.05×10^{-5}[d]
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	No data	No data	90[c]
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[e]	1 mg/m^3=0.054 ppm	1 mg/m^3=0.048 ppm	1 mg/m^3=0.049 ppm
Explosive limits	No data	No data	No data

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids[a]

Property	Permethrin	Phenothrin	Resmethrin
Molecular weight[c]	391.3	350.5	338.4
Color	Colorless to yellow[c]	Colorless	Colorless
Physical state	Crystals to viscous liquid[c]	Liquid	Crystals
Melting point, °C	34–35	No data	56.5
Boiling point, °C	220 at 0.05 mm Hg[f]	>290	Dec. at >180 °C
Density, g/cm^3 at 25 °C	1.19–1.27 (20 °C)	1.061	0.96-0.97 (20 °C)
Odor	No data	No data	Chrysanthemate
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	0.006 (20 °C)	2.0 (30 °C)	0.037 (25 °C)[b]
Organic solvent(s)	Soluble	Soluble	Soluble
Partition coefficients:			
Log K_{ow}	6.5	7.54[f]	5.43
Vapor pressure, mm Hg at 25 °C	$2.2x10^{-8}$	$1.4x10^{-7}$[b]	$1.13x10^{-8}$[i]
Henry's Law constant, atm-m^3/mol at 25 °C	$1.9x10^{-6}$[d]	$1.4x10^{-6}$[f]	$<8.9x10^{7}$[d]
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens closed cup)	>100[b]	107[b]	129[b]
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[e]	1 mg/m^3=0.062 ppm	1 mg/m^3=0.070 ppm	1 mg/m^3=0.072 ppm
Explosive limits	No data	No data	No data

Table 4-5. Physical and Chemical Properties of Selected Pyrethroids[a]

Property	Tefluthrin[b]	Tetramethrin	Tralomethrin
Molecular weight	418.7	331.4	665.0
Color	Colorless	Colorless	Yellow orange
Physical state	Solid	Crystals	Resinoid
Melting point, °C	44.6	65–80	138–148
Boiling point, °C	153 at 1 mm Hg	180–190	No data
Density, g/cm^3 at 25 °C	1.48	1.1 (20 °C)	1.70 (20 °C)
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water, mg/L	0.002 (20 °C)	1.83[b]	0.08
Organic solvent(s)	Soluble	Soluble	Soluble
Partition coefficients:			
Log K_{ow}	6.5	4.6[c]	7.6[f]
Vapor pressure, mm Hg at 25 °C	6.0x10^{-5}	7.1x10^{-6}[b]	3.6x10^{-11}
Henry's Law constant, atm-m^3/mol at 25 °C	4.6x10^{-4}[f]	8.3x10^{-9}[f]	3.9x10^{-15}[d]
Autoignition temperature	No data	No data	No data
Flashpoint, °C (Pensky-Martens open cup)	124	No data	No data
Flammability limits, °C	No data	No data	No data
Conversion factors			
Air (25 °C1)[g]	1 mg/m^3=0.058 ppm	1 mg/m^3=0.074 ppm	1 mg/m^3=0.074 ppm
Explosive limits	No data	No data	No data

[a]All information obtained from HSDB 2001 except where noted
[b]Tomlin 1997
[c]Technical grade
[d]USDA 2001a
[e]Milne 1995
[f]Estimated value from EPIWIN (Syracuse Research Corporation)
[g]These air conversion factors were calculated by using the average molecular weight and ideal gas law
[h]Budavari 1996
[i]Howard and Meylan 1997

Figure 4-2. Illustration of the S Conformer about the Alpha Carbon for the Type II Pyrethroid Cyhalothrin