

SPEX CertiPrep App Note

History of Pesticides and Pesticide Solubility

Modern pesticides are a product of the birth of the first synthetic organic chemicals (organochloride compounds) in the late 19th and early 20th centuries. Many organochloride compounds, such as BHC and DDT, were first synthesized in the 1800s; but their properties as insecticides were not fully discovered and exploited until the late 1930's. The organochloride class of pesticides grew out of those initial discoveries and, through the 1930's-1970's, developed into the range of organochloride pesticides known today.

Primarily, there are two groups of organochloride pesticides: chlorinated alicyclic and cyclo diene compounds (aldrin, dieldrin, endrin, heptachlor, chlordane, and endosulfan), and the DDT compounds (DDD, DDE, etc.). The discovery of DDT for pesticide use was a huge boon to the war efforts. Prior to the discovery of DDT, pyrethrins were one of the major insecticides in use. However, pyrethrins were extracted from natural sources, primarily from flowers of the genus *Chrysanthemum* (*Pyrethrum*), supplies of which were limited and could not meet demands of wartime needs.

At the time, DDT was seen as a broad spectrum insecticide with low toxicity to mammals. DDT targets the peripheral nervous system of invertebrates and is insoluble in water and therefore was not washed away by weather making reapplication unnecessary. Early pesticide development saw limited solubility in water and persistence as beneficial traits in a pesticide. It allowed the pesticide to stay where it was applied for a long period of time. These traits also allowed bioaccumulation over the decades in highly soluble lipid tissues of higher animals.

By 1945, DDT was made available for agricultural applications. By the 1950's, the first signs of insect resistance to DDT began to appear. DDT was in widespread use around the world until the 1970's and 1980's. The EPA canceled most uses of DDT by 1972 due to impact of bioaccumulation on higher animals and the environment. Many other countries shortly followed suit by removing DDT from most agricultural applications.

Since the start of the production boom in the 1940's to present day, a huge catalog of thousands of insecticides, herbicides, and general pesticides was developed, including organochlorides (DDT, BHC), organophosphates (parathion, malathion, azinphos methyl), carbamates (aldicarb, carbofuran, etc.), and neonicotinoids (imidacloprid & acetamiprid). As modern pesticides develop there has been a shift to understand and apply the chemical properties and interactions of pesticides with both the environment and animals other than the target pests. Early pesticides were, for the most part, persistent chemicals that affected the nervous system of invertebrates. These pesticides had, in many cases, limited solubility and persisted for years or decades after delivery. More modern pesticides take into consideration the half-life of pesticides and how they degrade in the environment.

One of the more modern developments in the pesticide arsenal is the synthetic nicotinoids and neonicotinoids. These pesticides are neuro-active insecticides, similar to nicotine compounds, and were developed in the 1980's and 1990's. Of all of the neonicotinoids, imidacloprid has become one of the most abundantly used insecticides in the world. Imidacloprid works by disrupting the transmission of nerve impulses in insects by binding to an insect's nicotine acetylcholine receptors in paralysis and death of the insect. Imidacloprid is highly toxic to insects and other arthropods, including marine invertebrates. It is considered to be moderately toxic to mammals, if ingested at high dosages. The acute toxicity and environmental fate of imidacloprid and other neonicotinoid pesticides have been greatly debated since their adaptation in the 1990's. Many studies question the persistence of neonicotinoids in water supplies and the ecological impacts to other environmentally and economically important arthropods.

Chemical pesticides are now an integral part of the world's agricultural arsenal, offering protection to crops from destructive pests. However, some disastrous side effects of their use include probable leaching of these often harmful chemicals into the environment and their ultimate presence in the human food chain. Because of this, pesticide residue analysis has become a serious testing process for several different types of laboratories. Each pesticide group in historical or modern use has their own set of physical and chemical properties which can make pesticide analysis a challenge. Some pesticides have low solvent solubility, making them difficult to place in solution (see Pesticide Chemical Property Tables below). Other pesticides degrade at lower temperatures which makes them only amenable to specific analytical applications such as LC/MS. SPEX CertiPrep has compiled the common properties and solubilities for the most common pesticide groups in order to aid in your pesticide analysis.

History of Pesticides and Pesticide Solubility

≥ 1000	Excellent Solubility
< 1000	Good Solubility
< 500	Moderate Solubility
< 100	Low Solubility
< 10	Insoluble

Red text – SPEX data shows minimum solubility @ 1,000 µg/mL
 Yellow text – Minimum solubility based on similar solvents cited
 N/D – No Data

Pyrethroids

	Water	Acetone	Methanol	Acetonitrile	Ethyl Acetate	Methylene Chloride	n-Hexane
MW	18.02	58.05	32.04	41.05	88.11	84.93	86.18
UV cutoff (nm)	200	330	205	190	260	235	200
BP (°C @ 1 atm)	100.0	56.1	64.7	81.6	77.1	39.5	69.0
Polarity index (Snyder)	9.0	5.1	5.1	5.8	4.4	3.1	0.0
Viscosity (cP)	1.00	0.32	0.60	0.37	0.45	0.44	0.33
Solubility in Water (% wt/wt)	100 %	100%	100%	100%	9%	2%	0%

Compound	CAS #	MW	Class	Molecular Formula	BP (°C @ 1 atm)	MP (°C @ 1 atm)	Density (g/cm ³ @ 20°C)	Color	Form	Solubility						
Bifenthrin	82657-04-3	422.9	Insecticide	C ₂₃ H ₂₂ ClF ₃ O ₂	Decomposes	80 °C	1.26	Off-White to Brown	Semi-Solid or Liquid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Cyfluthrin	68359-37-5	434.3	Insecticide	C ₂₂ H ₁₈ Cl ₂ F-NO ₃	Decomposes	79 °C	1.28	Yellow to Brown	Semi-Solid or Liquid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Cypermethrin	52315-07-8	416.3	Insecticide	C ₂₂ H ₁₉ Cl-2NO ₃	Decomposes	41 °C	1.25	Yellow	Crystalline or Waxy Solid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Etofenprox	80844-07-1	376.5	Insecticide	C ₂₅ H ₂₈ O ₃	Decomposes	37 °C	1.17	White	Crystalline Solid	<10	≥1000	≥1000	≥1000	≥1000	N/D	N/D
Fenpropathrin	39515-41-8	349.4	Acaricide	C ₂₂ H ₂₃ NO ₃	N/D	47 °C	1.15	Yellow to Brown	Oily Liquid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Fenvalerete	51630-58-1	419.9	Insecticide	C ₂₅ H ₂₂ ClNO ₃	Decomposes	39 °C	1.18	Yellow to Brown	Crystalline or Waxy Solid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Permethrin (mix of isomers)	52645-53-1	391.3	Insecticide	C ₂₁ H ₂₀ Cl ₂ O ₃	200 °C	34 °C	1.29	Colorless to Brown	Oily Liquid or Crystals	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Prallethrin (mix of isomers)	23031-36-9	300.4	Insecticide	C ₁₉ H ₂₄ O ₃	313 °C	-25 °C	1.03	Yellow to Brown	Oily Liquid	<10	≥1000	≥1000	≥1000	≥1000	N/D	≥1000
Pyrethrin (mix of isomers)	8003-34-7	328.4	Insecticide	C ₂₁ H ₂₈ O ₃	N/D	142 °C	0.85	Yellow to Brown	Oily Liquid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000
Resmethrin (mix of isomers)	10453-86-8	338.4	Insecticide	C ₂₂ H ₂₆ O ₃	Decomposes	56 °C	0.96	Colorless to Tan	Oily Liquid or Crystals	<10	≥1000	≥1000	≥1000	≥1000	≥1000	N/D
Tetramethrin	7696-12-0	331.4	Insecticide	C ₁₉ H ₂₅ NO ₄	N/D	69 °C	1.11	Colorless	Crystalline Solid	<10	≥1000	≥1000	≥1000	≥1000	≥1000	≥1000

Contact Us

Phone: 800.LAB.SPEX • 732.549.7144 • Fax: 732.603.9647
 CRMSales@spex.com • spexcertiprep.com

© 2020 SPEX CertiPrep. All Rights Reserved.

