# Semester-VI17CHU604BPESTICIDE CHEMISTRY3H3CInstruction Hours/week: L:3 T:0 P:0Marks: Internal: 40 External: 60 Total:100

#### Scope

The course involves the synthesis and manufacture of diverse pesticides

#### Objectives

The course enables the students to

- 1. Understand the synthesis and manufacture of many natural and synthetic fertilizers
- 2. Understand the synthesis and manufacture of organochlorines and organophosphorous compounds
- 3. Understand the synthesis and manufacture of quinine pesticides

#### 4.

#### Methodology

Blackboard teaching, Powerpoint presentation and group discussion.

#### Unit I

General introduction to pesticides (natural and synthetic), benefits and adverse effects.

#### Unit II

Changing concepts of pesticides, structure activity relationship.

#### Unit III

Synthesis and technicalmanufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,)

#### Unit IV

Synthesis and technicalmanufacture and uses of Organophosphates (Malathion, Parathion ); Carbamates (Carbofuranand carbaryl)

#### Unit V

Synthesis and technicalmanufacture and uses of Quinones ( Chloranil), Anilides (Alachlor and Butachlor).

#### **Suggested Reading**

T1: H.Ohkawa ,H.Miyagawa,P.W.Lee, Pesticide Chemistry, Wiley-VCH,2007,ISBN: 978-3-527-31663-2



#### KARPAGAM ACADEMY OF HIGHER EDUCATION

(Deemed to be University)

(Established Under Section 3 of UGC Act 1956)

Coimbatore - 641 021.

(For the candidates admitted from 2017 onwards)

#### **DEPARTMENT OF CHEMISTRY**

#### **SUBJECT NAME: Pesticide Chemistry**

SUBJECT CODE: 17CHU604B

**SEMESTER: VI** 

CLASS: III B.Sc CHEMISTRY

#### LECTURE PLAN

#### **DEPARTMENT OF CHEMISTRY**

S.No	Lecture Hour	Topics to be Covered	Support Materials/Page Nos
		UNIT I	
1.	1	General introduction to pesticides	T1:13
2.	1	Natural pesticides	T1:16
3.	1	Synthetic pesticides	T1:17
4.	1	Types of pesticide	T1:18
5.	1	Benefits and adverse effects of pesticides	T1:103
6.	1	Revision and discussion	
	Total No o	f Hours Planned For Unit I = 6	
		UNIT II	
1.	1	Introduction about Changing concepts of pesticides	T1:127
2.	1	Types or various Changing concepts of pesticides	T1:130

3.	1	Changes in pesticide manufacturing attitude	T1:132
4.	1	Changing patterns in pesticide use	T1:133
5.	1	Structure activity relationship	T1:128
6.	1	Revision and discussion	
<b>Total</b>	No of Hour	s Planned For Unit II = 6	
		UNIT III	
1.	1	Introduction about Organochlorines	T1:127
2.	1	Synthesis of DDT	T1:305
3.	1	Synthesis of Gammexenes	T1:306
4.	1	General manufacturing process of DDT and Gammexenes	T1:308
5.	1	Uses of DDT and Gammexenes	T1:309
6.	1	Revision and discussion	
	Total No o	of Hours Planned For Unit III = 6	
		UNIT IV	
1.	1	General introduction about Organophosphates and Carbamates	T1:340
2.	1	Synthesis and uses of Malathion	T1:419
3.	1	Synthesis and uses of Parathion	T1:231
4.	1	Synthesis and uses of Carbofuran	T1:342
5.	1	Synthesis and uses of carbaryl	T1:343
6.	1	Revision and discussion	
	Total No o	of Hours Planned For Unit IV =6	

	UNIT V						
1.	1	General introduction about Quinones	T1:172				
2.	1	Synthesis, manufacture and uses of Chloranil	T1:329				
3.	1	Synthesis, manufacture and uses Alachlor	T1:340				
4.	1	Synthesis, manufacture and uses Butachlor	T1:342				
5.	1	Application of Quinones	T1:174				
6.	1	Revision and discussion of ESE question papers					
	Total No	o of Hours Planned For Unit I =6					

#### **SUPPORTING MATERIALS:**

#### Text books:

T1: H.Ohkawa ,H.Miyagawa,P.W.Lee, Pesticide Chemistry, Wiley-VCH,2007,ISBN: 978-3-527-31663-2



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CLASS: III- B.SC CHEMISTRY COURSE CODE:17CHU604B

### COURSE NAME: PESTICIDE CHEMISTRY UNIT-I BATCH: 2017-2020

#### Unit I

General introduction to pesticides (natural and synthetic), benefits and adverse effects.

#### Pesticides

Pesticides are chemical substances that are meant to kill pests. In general, a pesticide is a chemical or a biological agent such as a virus, bacterium, antimicrobial, or disinfectant that deters, incapacitates, kills, pests.

#### **A Brief History**

Pesticides are not recent inventions! Many ancient civilizations used pesticides to protect their crops from insects and pests. Ancient Sumerians used elemental sulfur to protect their crops from insects. Whereas, Medieval farmers experimented with chemicals using arsenic, lead on common crops.

The Chinese used arsenic and mercury compounds to control body lice and other pests. While, the Greeks and Romans used oil, ash, sulfur, and other materials to protect themselves, their livestock, and their crops from various pests.

Meanwhile, in the nineteenth century, researchers focused more on natural techniques involving compounds made with the roots of tropical vegetables and chrysanthemums. In 1939, Dichloro-Diphenyl-Trichloroethane (DDT) was discovered, which has become extremely effective and rapidly used as the insecticide in the world. However, twenty years later, due to biological effects and human safety, DDT has been banned in almost 86 countries.

#### **Definition of Pesticides**

#### The Food and Agriculture Organization (FAO) has defined pesticide as:

any substance or mixture of substances intended for preventing, destroying, or controlling any pest, including vectors of human or animal disease, unwanted species of plants or animals, causing harm during or otherwise interfering with the production, processing, storage, transport, or marketing of food, agricultural commodities, wood and wood products or animal feedstuffs, or



substances that may be administered to animals for the control of insects, arachnids, or other pests in or on their bodies.

#### What are natural pesticides?

Natural pesticides are pesticides that are made by other organisms usually for their own defense, or are derived from a natural source such as a mineral or plant. ... Plants produce many natural pesticides that they use for their own defense against insects and disease organisms.

**Synthetic Insecticides.** Pesticides are products designed to kill certain organisms. An insecticide is a pesticide formulated to kill insects. Chemical insecticides, both "organic" (of natural origin) and man-made or synthetic products continue to be the main method of battling insect pests of ornamental plants.

Some examples of organic pesticides, i.e. pesticides acceptable for organic agriculture, include some are household detergents, pyrethrin, lime sulfur, sabadilla, garlic, onions, ryania, tomato leaves (crushed), tobacco water, snuff, retenone, oil and sulfur sprays, talcum powder, soapsuds, rhubarb leaves, garlic and

#### **Types of Pesticides**

Insecticides – insects.

Herbicides – plants.

Rodenticides – rodents (rats & mice)

Bactericides - bacteria.

Fungicides – fungi.

Larvicides - larvae.

#### Chemically-related pesticides:

#### **Organophosphate:**

Most organophosphates are insecticides, they affect the nervous system by disrupting the enzyme that regulates a neurotransmitter.

#### **Carbamate:**

Similar to the organophosphorus pesticides, the carbamate pesticides also affect the nervous system by disrupting an enzyme that regulates the neurotransmitter. However, the enzyme effects are usually reversible.



#### **Organochlorine insecticides:**

They were commonly used earlier, but now many countries have been removed Organochlorine insecticides from their market due to their health and environmental effects and their persistence (e.g., DDT, chlordane, and toxaphene).

#### **Pyrethroid:**

These are a synthetic version of pyrethrin, a naturally occurring pesticide, found in chrysanthemums(Flower). They were developed in such a way as to maximise their stability in the environment.

#### Sulfonylurea herbicides:

The sulfonylureas herbicides have been commercialized for weed control such as pyrithiobac-sodium, cyclosulfamuron, bispyribac-sodium, terbacil, sulfometuron-methyl Sulfosulfuron, rimsulfuron, pyrazosulfuron-ethyl, imazosulfuron, nicosulfuron, oxasulfuron, nicosulfuron, flazasulfuron, primisulfuron-methyl, halosulfuron-methyl, flupyrsulfuron-methyl-sodium, ethoxysulfuron, chlorimuron-ethyl, bensulfuron-methyl, azimsulfuron, and amidosulfuron.

#### **Biopesticides:**

The biopesticides are certain types of pesticides derived from such natural materials as animals, plants, bacteria, and certain minerals.

#### **Examples of pesticides**

Examples of pesticides are fungicides, herbicides, and insecticides. Examples of specific synthetic chemical pesticides are glyphosate, Acephate, Deet, Propoxur, Metaldehyde, Boric Acid, Diazinon, Dursban, DDT, Malathion, etc.

#### **Benefits of Pesticides**

The major advantage of pesticides is that they can save farmers. By protecting crops from insects and other pests. However, below are some other primary benefits of it.

- Controlling pests and plant disease vectors.
- > Controlling human/livestock disease vectors and nuisance organisms.
- > Controlling organisms that harm other human activities and structures.

#### **Effects of Pesticides**



The toxic chemicals in these are designed to deliberately released into the environment. Though each pesticide is meant to kill a certain pest, a very large percentage of pesticides reach a destination other than their target. Instead, they enter the air, water, sediments, and even end up in our food.

Pesticides have been linked with human health hazards, from short-term impacts such as headaches and nausea to chronic impacts like cancer, reproductive harm.

The use of these also decreases the general biodiversity in the soil. If there are no chemicals in the soil there is a higher soil quality, and this allows for higher water retention, which is necessary for plants to grow.

#### What are the harmful effects of pesticides?

Pesticides have been linked to a wide range of human health hazards, ranging from short-term impacts such as headaches and nausea to chronic impacts like cancer, reproductive harm, and endocrine disruption

#### What diseases can pesticides cause?

The common diseases affecting the public's health are all too well-known in the 21st century: asthma, autism and learning disabilities, birth defects and reproductive dysfunction, diabetes, Parkinson's and Alzheimer's diseases, and several types of cancer.

#### What is the most harmful pesticide?

That structure makes dichloropropene one of the simplest of a class of chemicals called organochlorines, which include some of the most toxic pesticides available. Banned as unsafe by the European Union, 1,3-dichloropropene is nevertheless one of the most commonly used pesticides in the United States.

#### What chemicals are in pesticides?

Pesticides (chemicals used for killing pests, such as rodents, insects, or plants)

2,4-Dichlorophenoxyacetic Acid (2,4-D)

Aldrin/Dieldrin.

Atrazine.

Chlordane.



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Chlordecone.

DDT, DDE, DDD.

Endosulfan.

Endrin (Endrin aldehyde)

#### What are the long term effects of pesticides?

Pesticides can cause short-term adverse health effects, called acute effects, as well as chronic adverse effects that can occur months or years after exposure. Examples of acute health effects include stinging eyes, rashes, blisters, blindness, nausea, dizziness, diarrhea and death.

#### What are methods of pest control?

#### **Control methods**

Biological pest control.

Cultural control.

Trap cropping.

Pesticides.

Physical pest control.

Poisoned bait.

Fumigation.

Sterilization.

S.	unit-1 QUESTIONS:	OPTION-A	OPTION-B	OPTION-C	OPTION-D	ANSWER
Ν						
0						
1	Pesticides is used to control	Bacteria	Insects	Weeds	Virus	Weeds
2	Insecticides is used to control	Insects	Bacteria	Virus	Weeds	Insects
3	Pesticides is used to control	Unwanted	Bacteria	Weeds	Virus	Uwanted
		Vegetation				vegetation
4	Fungicides is used to prevent	Bacteria	Molds and	Mice	Weeds	Molds and
			mildew			mildew
5	Disinfectants for prevention of	Bacteria	Molds and	Unwanted	Insects	Bacteria
			mildew	vegetation		
6	Pesticides used to protect	Plants	Bacteria	Molds	Insects	Plants
7	Herbicides is also called as	Insecticides	Fungicides	Pesticides	All the above	Pesticides
8	To control larvae is used	Rodenticides	Insecticides	Larvicides	Disinfectants	Larvicides
9	The example for synthetic pesticides	Glyphosate	Fungicides	Herbicides	Insecticides	Glyphosate
10	The example for natural pesticides	Herbicides	Acephate	Glyphosate	Boric acid	Herbicides
11	Pyrethirn is occuring from	Chrysanthemu	Suiphur	Organochlorine	Carbamate	Chrysanthemums
		ms				
12	Organophosphate are	Insecticides	Fungicides	Rotenticides	Larvicides	Insecticides
13	Example for organochlorine	Amidosulphur	Pyrethirn	DDT	None of these	DDT
		on				
14	The naturally occuring pesticides found	Pyrethirn	DDT	Sulphur	Carbamate	Pyrethirn
	in chrysanthemums					
15	An example for sulphonylurea	Amidosulphur	Carbamate	DDT	Pyrethirn	Amidosulphuron
	herbicides	on				
16	Sulphonylurea is	Carbamate	Herbicides	Insecticides	None of these	Herbicides
17	Toxaphene is	Organochlorin	Organophosphate	Organic	Carbamate	Organochlorine
	_	e		chemical		
18	Chlordane is	Fungicides	Insecticides	Rotenticides	Larvicides	Insecticides

19	Organophosphate affect	Nervous	Respiratory	liver	lungs	Nervous system
		system	system			
20	Carbamate affect	Respiratory	Nervous system	Liver	Lungs	Nervous system
		system				
21	The nervous system is affected by	Organochlorin	Organophosphate	Carbamate	Both b and c	Both b and c
		e				
22	The type of pesticides that derive from	Bioinsecticide	Fungicides	Biopesticides	larvicides	Biopesticides
	natural material are	S				
23	Biopesticides are derived from	Plants and	Bacteria only	Plants only	Fungai only	Plants and
		Bacteria				Bacteria
24	Boric acid is	Pesticides	Fungicides	Larvicides	Certain	Pesticides
					mineral	
25	Ancient sumerians are used	Chlorine	Sulphur	Phosphorus	Arsenic	Sulphur
	element to protect crops					
26	FAO	food	Food and	Field	None of these	Food and
		administrative	administrative	administrative		administrative
		organization.	organization	organization		organization
27	Pesticides can aso consider as	Biodegradable	Persistent only	Biodegradable	To kill insects	Biodegradable
		and Persistent		only		and Persistent
28	Terbacil is	Sulphonylurea	Organophosphate	Organochlorine	Carbamate	sulphonylurea
29	Dursban is	Organochlorin	Carbamate	Sulphonylurea	Synthetic	Synthetic
		e			pesticides	pesticides
30	DDT was discovered in	1940	1936	1938	1939	1939
31	Rotenticides is used to kill	Plants	Insects	None of these	Rat	Rat
32	DDT has banned in countries	76	66	96	86	86
33	DDT is a	Fungicides	Insecticides	Organochlorine	Carbamate	Insecticides
34	DDT is	Dichloro-	Dibromo-	Disulpho-	Difluro-	Dichloro-
		diphenyl-	diphenyl -	diphenyl -	diphenyl -	diphenyl-
		trichloroethan	trichloroethane	trichloroethane	trichloroethan	trichloroethane
		e			e	

35	Pesticides are impact of	Headaches	Nausea	Chronic	All the above	All the above
36	which is used to control pest in plants	Pesticides	Organisms	Insects	Birds	Pesticides
37	Metaldehyde is pesticides	Synthetic	Natural	Biopesticides	Persistant	Synthetic
38	Oxasulphuron is	Fungicides	Insecticides	Pesticides	Rotenticides	Insecticides
39	which is made with a root of tropical vegetables	Pyrethirn	Phosphates	Chrysanthemu ms	Sulphonylurea	Chrysanthemums
40	Diazinon is pesticides	Natural	Synthetic	Chemical	All the above	Chemical
41	By using pesticides the farmers are affected by	Chronic	Headache	Respiratory problems	All the above	Headache
42	There are types of pesticides	3	4	5	6	6
43	Which promotes the growth of the foliage	Sulphur	Nitrogen	Phosphorus	Potassium	Nitrogen
44	Which promotes the growth of the strond root, stem, flowers and fruits	Nitrogen	Phosphorus and Potassium	Potassium	Phosphorus	Phosphorus and Potassium
45	which affects the plant growth	Fertilizers	Insecticides	Heavy metals	Pesticides	Heavy metals
46	Azadirachtin is extracted from	Neem tree	Coconut tree	Banana leaf	None of these	Neem tree
47	Natural insecticides are	DDT	Boric acid	Nicotin	Oxasulphuron	Nicotin
48	Most widely used pesticides	Nicotin	DDT	Amidosulphuro n	Chlororpyrifo s	Chlororpyrifos
49	Chlororpyrifos was introduced by	Fermant	Dow chemical	Both a and b	None of these	Dow chemical
50	Dow chemical was introduced in	1963	1968	1965	1961	1965
51	Most toxic pesticides is	Chlororpyrifo s	Dichloropropene	Nicotin	Azadirachtin	Dichloropropene
52	Dow chemical is	Fertilizers	Dichloropropene	Chlororpyrifos	Sodium bis sulphate	Chlororpyrifos
53	From neem tree is extracted	Dichloroprope ne	Fertilizers	Chlororpyrifos	Azadirachtin	Azadirachtin
54	Nicotin is	Natural	Synthetic	Pesticides	Insecticides	Insecticides

55	The elements sulphur is used to protect	Ancient	Greeks	Romans	Chinese	Ancient
	crops by	sumerians				sumerians
56	The heavy metals are used to protect	Romans	Chinese	Sumerians	Greeks	Chinese
	crops by					
57	In agricultural field the pesticides are	19th century	17th century	16th century	20th century	19th century
	commonly used in					
58	The pesticides that derived from plants	Insecticides	Fungicides	Biopesticides	Pesticides	Biopesticides
	are					
59	Toxaphene is pesticides	Natural	Synthetic	Chemical	Natural and	Chemical
					Synthetic	
60	The molds and mildew are prevented by-	Insecticides	Fungicides	Pesticides	Rotenticides	Fungicides



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#### Unit II

Changing concepts of pesticides, structure activity relationship.

#### Changing concepts of pesticides:

The drawbacks most often cited with injudicious and indiscriminate use of pesticides include development of pest resistance to pesticides, destruction of natural enemies, poisoning of man and animals, environmental pollution, minor pest assuming major status and increasing costs etc. Then a change in the attitude of policy planners of pesticide use, researchers, pesticide manufacturers and users of pesticides was observed.

#### The following changes are needed in pesticide usage:

- Changes in Pesticide Policy and Legislation
- Change in Public Perception
- > Changes in Pesticide Manufacturing Attitude
- Change in Population
- > Availability of Practical IPM Programmes (Integrated Pest Management)
- Innovative Technologies
- Changing Patterns in Pesticide Use
- Future of Pesticide Use

#### **Changes in Pesticide Policy and Legislation**

Several international actions have been undertaken on pesticide use in developing countries. Such policies and legislation are aimed at improved pesticide management, a practice that can help avoid pesticide misuse and the possible loss of a valuable and badly needed pest control tactic in the third world. Food and Agricultural Organization (FAO)/ World Health Organization (WHO) established the Codex Alimentarius Commission in 1963 to harmonize international pesticide residue standards through legislation that affect shipment of food item. In India, the Directorate of Plant Protection, Quarantine and Storage organization was set up in 1946 under the Ministry of Agriculture, Government of India, which was later, shifted to Faridabad in 1968. This organization looks after the registration, banning, quality testing and setting up laws for pesticide use. Besides, some other laws enforced by Government of India to prevent environmental pollution are Environment Protection Act, 1968, Water (Prevention and Control of Pollution) Act, 1974 and Water Cess Act, 1977. As of this time, over 40 pesticides are included on the suspended, cancelled and restricted use list by Government of India.

#### **Change in Public Perception**

In spite of much intensified and restrictive requirements for registration of pesticides and a greatly accelerated programme for the reregistration of existing pesticides as well as substantial





scientific conclusions on pesticide safety, agricultural pesticides are still perceived as unacceptably hazardous to human health and the environment. These perceptions, added with pressure from environmentalists encourage the development of additional pesticide regulation. The resulting decline in available pesticide choices will severely limit not only chemical pest control options but also the flexibility they offer in terms of developing Integrated Pest Management (IPM) programmes. IPM is a subject to credibility with farmers. Farmers often receive distorted views of IPM as "pest control without synthetic chemical" or as "biological control" and as a result become reluctant to relinquish their pesticide oriented but dependable pest management programmes.

#### **Changes in Pesticide Manufacturing Attitude**

It is the older, less expensive chemical that are often used in developing countries and most of the pesticides those are obsolete or banned in developed countries are manufactured in developing countries without compliance with safety requirements or the production standards of the multinational companies.

Recent advances in the understanding of insect ecology, biology, physiology and biochemistry are providing new impetus and opportunities for insect pest control.

#### Changing Patterns in Pesticide Use

Synthetic pesticides have been extensively used in developing countries mostly after the adoption of green revolution and the

control of vector borne diseases. By the early 1980's the developing countries were thought to use 10 - 25% of the world pesticide production. However, about 1/3rd of the crops were still lost to pests each year and malaria alone affected 100 million people annually. By 1990, the third world countries used 26% of the world pesticide production. Around 55% of agricultural land situated in these countries is related to much lower consumption of pesticides than developed countries. Taiwan tops the list using 17 kg a.i./ha followed by Japan (12 kg a.i./ha) and Africa, the least with 0.13 kg a.i./ha, while India used 0.57 kg a.i./ha in the year 1998. Many developing countries including India, China, Bangladesh and Indonesia are participating in the global expansion of agricultural output. The value of pesticide imports to Asia increased three fold between 1970s to 1980s. The fastest growing pesticide markets are India, Brazil, China and Spain. Of the total world pesticide production 24% reach the developing countries, 12% goes to Asia, 8% to Latin America and 4% to Africa.

In India, the total amount of pesticides used in the country increased from 2.35 thousand metric tones in 1950-51 to nearly 85,000 metric tones in 1993-94. Earlier projections had put the pesticide demand by 2000 at nearly 1-lakh metric tones. But in view of the high priority being accorded to IPM, the pesticide consumption has shown a decreasing trend in the recent years. In Tamil Nadu the synthetic pesticide consumption has decreased by more than 50% during last 7 years, a decreasing trend has also been recorded in Andhra Pradesh and Karnataka. In contrast





pesticide consumption continues to rise rapidly in Punjab and Rajasthan. In 1992, the world consumption of herbicides was 44%, insecticides 30%, fungicides 20% and others 6% of the total pesticide consumption compared to 77% insecticides, 12% herbicides, 8% fungicides and 3% others in India. When cotton utilized 54%, rice 17%, cereals and millets 6%, and others 235 of total pesticide consumption in 1979 in India it was 39% in cotton, 35% in rice, 17% in cereals and millets and 9% in others in the year 1988. In contrast to this, 27% of the total pesticides were used in horticulture, 17% in rice, 24% in cotton, 7% in maize and 25% in others in the world in 1992. The world market on pesticides is estimated to grow @ 4.5% each year with the largest growth occurring in herbicides. The average growth rate in Asia Pacific region is approximately 5–7%, but in Indonesia and Pakistan, the market is expanding @ 20-30% per annum. Along with the increase in the amount of pesticide consumption, there is a change in the potency of some new chemicals observed in recent past. DDT was applied @ 1-2kg a.i./ha for the control of different pests, the organophosphates in general are effective @ 250-500 g a.i./ha, synthetic pyrethroids @ 12.5- 100 g a.i./ha. Some recently developed chemicals like nitroguanidines are effective @ 25 g a.i./ha. Thus there has been more than 100-fold increase in the potency of new insecticides.

#### **Future of Pesticide Use**

The future of pesticide use in IPM is expected to depend on the continuation of existing pest management tactics and technology including the use of pesticides. Although the present environmentally conscious society rules out the placement of pesticides in IPM but it is technically correct for the pesticides to find a place, may be as the last alternative of IPM. The pesticide industries should orient towards

- i) lower margins,
- ii) financing IPM research and extension in countries where national institutes are weak, utilizing their marketing skills in the promotion of IPM and
- iii) organizing smallscale farmers so that they can benefit from

knowledge as much as the large scale farmers. The direction of pesticide development should be clearly in the direction of developing low risk materials. It may be necessary to create special situations whereby the high-risk materials may be used in special situations in special manner, placing them in a "prescriptive" use category.

#### Structure-Activity Relationships (SAR):

The study on the relationships between molecular structure and physicochemical and biological response, collectively known as Structure-Activity Relationships (SAR), is a rapidly growing field of research in chemistry and biology. Some areas of the application of SAR include the design of more active and less toxic agricultural products (Martin 1978).

Basically, a SAR analysis consists of comparison between experimental values by mathematical variance analysis (e.g. regression analysis, discriminant analysis, factorial analysis and pattern

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recognition techniques) and a selection of the best correlation values. The best-fitted correlations are then used to develop a mathematical expression to estimate end-values from known substances to unknown substances.

When performing a SAR analysis, it is assumed that the chemical or biological response produced by a substance (usually an organic compound) is a direct function of its chemical structure, and that the same substance will always produce the same response, under a given set of experimental conditions.

However, "chemical structure" cannot be dealt with directly. Instead quantities, usually of a numerical nature, which are derived from and represent the chemical structures, are used. These quantities are called molecular descriptors.

The molecular descriptors are of various types:

- fragments (e.g. counts of atoms, bonds of various types, rings, ring atoms, molecular weight)
- topological (e.g. molecular connectivity, molecular symmetry)
- geometrical (e.g. molecular surface area and volume)
- physico-chemical (e.g. molar refraction, log Kow) or substructural (e.g.topological)
- physico-chemical properties of substructures as embedded in the structure).

SAR is based on the knowledge that substances with a similar (analogous) chemical structure may have the same biological activity. SAR is a qualitative comparison of the structures of chemical compounds and their effects in the biological system. From this evaluation of the influence of the chemical structure on the biological system, combined with experience in how changes in the chemical structure affect the magnitude and type of biological effect, unknown toxic effects to the biological system of unknown compounds with related chemically structure are predicted.

#### **Quantitative Structure Activity Relationships:**

QSAR is a statistical data analytical procedure in which quantitative endpoints of compounds (e.g. toxicity) are correlated with one or more structural parameters of these compounds, normally through uni- or multivariate linear regression , non-linear regression (1981), bilinear (1983) or exponential regression. Commonly used structural parameters for inclusion in QSAR correlations are for instance:

- octanol-water partition coefficients (log Kow)
- aqueous solubility (log S)
- Molar Refraction or Parachor (dispersion forces)
- dipole moment
- ionisation potentials
- molar volumes
- molar surface areas (Hermens 1989).



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BATCH: 2017-2020

#### The scope of the structure-activity based modelling, the following parameters are considered:

- physico-chemical properties
- the partitioning of pesticides among environmental compartments
- bioaccumulation potential
- aquatic toxicity

#### **QSAR** modelling

A QSAR model is a mathematical expression that relates the variation of the biological activity in a series of structurally similar compounds to the variation in their chemical structure. Thus, a QSAR model is a mathematical equation describing the activity for a specific class of substances and derived from the quantified measured data belonging to these substances.

QSAR was previously used in the chemical industry in the development of new substances and only within the last decade the models have been refined to the use in assessment of chemical substances effects, fate and behaviour in the environment.

The American Environmental Protection Agency (US-EPA) has developed a system of QSARs which are connected to a database (AQUIRE) and can therefore use the latest evaluated endpoint-values, whether physico-chemical, effect or fate data. This should improve the models as the reliability of model estimations relies on the precision of the input data. The model system is called ASTER: Assessment Tools for the Evaluation of Risk (Russom 1991, Pedersen et al. 1995).

#### Thus, QSARs can be used to assist data evaluation

• to contribute to the decision on whether further testing is necessary to clarify an endpoint of concern

• to establish input parameters which are necessary to conduct the exposure or effect assessment.

#### Environmental risk assessment is based on a comparison of two variables:

• the concentration of the chemical in the environment (exposure)

• the concentration of the chemical at which no adverse effects on the environment are expected or estimated to occur.

#### A few physico-chemical parameters and variables are observed to be important, i.e.:

- the size and structure of the chemical
- the water solubility
- vapour pressure
- octanol/water partition coefficient (lipophilicity)
- adsorption coefficient.

#### The concentration, at which a chemical exerts an effect, depends on:

its toxicokinetic behaviour



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CLASS: III- B.SC CHEMISTRY COU COURSE CODE:17CHU604B UNIT-II

COURSE NAME: PESTICIDE CHEMISTRY
BATCH: 2017-2020

- uptake
- biotransformation
- distribution
- excretion/elimination
- its toxicodynamic behaviour
- interaction with receptor target

The development of QSAR is based on the assumption that chemical substances, which reach and interact with a target site by the same mechanism, perform likewise due to their similar chemical properties.

#### **Effect concentration**

The analysis for QSAR is through regression method affording transparent relations and simple mathematical equations and leading to a quantitative correlation. However, for a meaningful regression analysis, precise and accurate input data are required which tend to limit the number of samples in the testing set. It also means that the data used should be carefully evaluated and not taken from any available handbook unless the data quality is known to be validated (Hart 1991)

The QSAR estimations on physico-chemical proportions are performed by programmes developed by Syracuse Research Corporation: MPBPVP, WSKOW, KOWWIN, HENRY, and PCKOCWIN. The programmes are stand-alone programmes but can be run together using the Estimation Programs Interface (EPIWIN) as an interface. The programmes require that the molecular structure be presented as a SMILES notation,

#### **SMILES notation**

Simplified Molecular Input Line Entry System (SMILES) is a simple chemical notation system to identify the molecule from its structure by a linear string of symbols. The system has been designed so that a computer can use it. The chemical structure is described from basal symbols and a few rules:

- The SMILES notation can begin at any atom in the molecular structure.
- Hydrogen atoms are not presented.
- Normal atoms are named by capital letters (C, O, N, S, P...) unless they are included in aromatic ring structures.
- Aromatic atoms are named by small letters (c, o, n, s).
- Single bonds are not shown, double bonds as "=" and triple bonds as "#".

• Branches are presented in brackets. A branch cannot begin a SMILES notation but must follow immediately after the atom to which it connects. If an atom has more than one branch, the branches are coded as consecutive pairs of parentheses.



• Ring structures are numbered to identify which atoms that are connected to present the ring structure, e.g. benzene: c1ccccc1, 1,3,5-triazin: c1ncncn1 (Lagersted 1987). More rings are introduced by increasing number.

Examples of SMILES notation.

Eksempler på SM	ILES notation.	
Substance	Structure	SMILES
Isobutyric acid	н,с он	CC(C)C(-O)O or C(C)(C)C(-O)O or OC(-O)C(C)C or O-C(O)C(C)C
Benzene	$\bigcirc$	clocecc1
Triallate		CC(C)N(C(C)C)C(-O)SCC(CL)-C(CL)CL
Atrazine		n(c(nc(n1)NC(C)C)NCC)c1CL
Fenpropathrin		C1(C)(C)C(C)(C)C1C(-O)OC (C(#N))c2cccc(Oc3ccccc3)c2
Thifensulfuron- methyl	"Here	nlc(C)nc(OC)nc1NC(=O)NS(=O) (=O)c2ccsc2C(=O)OC

S.No	unit-2 QUESTIONS:	OPTION-A	OPTION-B	OPTION-C	OPTION-D	ANSWER
1	Which is nerotoxic chemical	Organochlorine	Carbamate	Sulphonylurea	Organophosphate	Organochlorine
2	DDT is type of	Brominated	Iodinated	Chlorinated	Flurinated	Chlorinated
		alicylices	alicylices	alicylices	alicylice	alicylice
3	Which affect biological activity	Electronic factor	Steric factor	Molecular	Shape	Electronic factor
4			т ·	volume		<b>.</b> .
4	Which is influenced in toxicity affect	Steric factor	Isomeric	Steric factor	Molucular	Isomeric
_			configuration		volume	configuration
5	Example for organochlorine is	Amidosulphuron	Dichloropropene	Aldrin	Pyrethroids	Aldrin
6	How many types of organochlorine are	1	2	3	4	2
7	Chlorinated alicyclic insecticides are	Dieldrin	DDT	Amidosulphuron	Dichloropropene	Dieldrin
8	Which compound have phenyl ring in	Amidosulphuron	Dieldrin	DDT	None of these	DDT
	it					
9	Which is four polychlorocycloalkane	Lindane	Heptachlor	Dieldrin	All the above	All the above
10	Which is naturally occuring ester	Lindane	Allethrin	Phenothrin	Dieldrin	Allethrin
11	Among which pesticides is used highly	Fungicides	Larvicides	Rotenticides	Herbicides	Herbicides
12	How many percentage of herbicides is used	96%	76%	86%	85%	86%
13	How many percentage of convientional pesticides used	80%	60%	50%	90%	80%
14	How many percentage of insecticides is used	40%	17%	15%	10%	17%
15	How many percentage of fungicides is used	40%	17%	15%	10%	10%
16	How many percentage of pesticides is used	40%	17%	15%	10%	40%

17	Which is polychlorocycloalkane	Lindane	ethylene	propene	propylene	Lindane
18	Which pesticides based on	Natural	Synthetic	Biological	Biopesticides	Biological
	entomopathogenic					
19	Which is entomopathogenic	Plants	Animals	Chemical	Fungi	Fungi
20	Among which is entomopathogenic	Viruses	Plants	Animals	Plants and	Viruses
					animals	
21	Among which is not	Viruses	Bacteria	Parasities	Fungi	Parasites
	entomopathogenic					
22	IMP IS	Integrated pest	Individual pest	Involving pest	Intimate pest	Integrated pest
		management	management	management	management	manage
23	Which is reduce plant-parasite	Carbon	Nitrogen	Carbon and	Sulphur	Carbon and
	nematodes			Nitrogen		Nitrogen
24	Among the following which is	Nematodes	Bacteria	Viruses	Fungi	Nematodes
	parasites					
25	Which is biopesticides	Sulphur	Natural material	Soil	None of these	Natural material
26	Microbial pesticides consist of	Fungi	Viruses	Nematodes	Bacteria	Bacteria
27	Among the following which affect	Birds	Rats	Pesticides	All the above	Pesticides
	soil					
28	Target pest include	Bacteria	Molluses	Birds	Mammals	Molluses
29	Nematodes are	Round worm	Ring worm	Tap worm	Molluses	Round worm
30	To control nematodes which is used	Molluscicides	Insecticides	Rotenticides	Nematicides	Nematicides
31	To control birds which is used	Nematicides	Fungicides	Avicides	None of these	Avicides
32	To control snails which is used	Avicides	Molluscicides	Nematicides	Rotenticides	Molluscicides
33	To control algae which is used	Nematicides	Bactericides	Fungicides	Algicides	Algicides
34	To control bacteria which is used	Bactericides	Algicides	Herbicides	Avicides	Bactericides
35	To control slime molds which is used	Bactericides	Algicides	Slimicides	Acaricides	Slimicides
36	To control mites which is used	Algicides	Miticides	Slimicides	Fungicides	Miticides
37	Miticides is also called as	Algicides	Acaricides	Fungicides	Miticides	Acaricides
38	Algicides is also known as	Algaecides	Acaricides	Fungicides	Miticides	Algaecides
39	Plant derived pesticides	Strychnine	Scilliroside	Rotenoids	Fumigant	Rotenoids
40	Among which is plant derived	Rotenoids and	Scilliroside	Nicotiniods	Rotenoids	<b>Rotenoids and</b>

	pesticides	Nicotiniods				Nicotiniods
41	EPA	Evolution of	Environmental	Environmental	Evolution of	Environmental
		pesticide agency	protection	pesticides agency	protection	protection
			agency		agency	agency
42	Whate are pesticides regulation	EPA	PMRA	EPA and PMRA	FAO	<b>EPA and PMRA</b>
	agency					
43	Slimicides is used to control	Slime mold and	viruse only	Algae only	Slime mold only	Slime mold and
		Algae	~	~		Algae
44	Which pesticides is used to control	Amidosulphuron	Glyphosate	Sulphonoylurea	Pyrethroids	Glyphsate
45	Weeds		D	01 1	• 1	
45	DDT is no longer effective in	Malaria	Dengue	Cholera	viral	Malaria
16	Disadvantage of using posticide is	Increase the soil	Ground water	Decrease the	Increase the	Ground water and
40	Disadvantage of using pesticide is	nature	and Quality of	pollution	crops	Quality of crops
		hatare	crops decrease	politicion	crops	Quality of crops
47	Use of pesticide can be control	Control pest	Increase in pest	No change	Increase in	Control pest
			F	8-	insects	Control Pros
48	Algicides is used to control	Bacteria	Fungi	Algae	Molds	Algae
49	Plant derived pesticides	Strychnine	Scilliroside	Acaricides	Nicotinoids	Nicotinoids
50	Organochlorine is a	Insecticides	Neurotoxic	Fungicides	All the above	Neurotoxic
			chemical			chemical
51	Aldrin is a	Carbamate	Sulphonoylurea	Organochlorine	Pyrethroids	Organochlorine
52	Heptachlor is a	Organochlorine	Carbamate	Organophosphate	DDT	Organochlorine
53	Miticides is used to prevent	Algae	Mites	Slime mold	Bacteria	Mites
54	Pesticides is used to control	Molds	Algae	Birds	Pest	Pest
55	Which is biological agent	Bacteria	ADP	ATP	HCl	Bacteria
56	To control viruses	Miticides	Virucides	Slimicides	Rotenticides	Virucides
57	Structural relationship activity is	Chemical	Biological	Chemical	Chemical and	Chemical
	between	structure and	activity only	structure only	Physical	structure and
		Biological			properties	Biological
		activity				activity
58	Molecular structure and their	MOE	MOT	CFT	Spectroscopy	MOE

	biological activities are done by					
59	Glyphosate is a	Organochlorine	Carbamate	Synthetic	Natural	Synthetic
60	Biological activites are held by	Biological agent	Chemical agent	Natural material	None of these	<b>Biological agent</b>



#### KARPAGAM ACADEMY OF HIGHER EDUCATION

CLASS: III- B.SC CHEMISTRY COURSE CODE:17CHU604B COURSE NAME: PESTICIDE CHEMISTRY
UNIT-III BATCH: 2017-2020

#### Unit III

Synthesis and technicalmanufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,)

#### **DDT:**

DDT is the abbreviation for p,p-dichlorodiphenyltrichloroethane and it is probably the compound, above all others, that first sparked off concern for the possible adverse effects of chemicals on the environment.

Synthesis of DDT:



1. DDT is dichlorodiphenyltrichloroethane

2. Organochlorines are chemical compounds that contain hydrogen, carbon, chlorine, and, sometimes, other atoms.

- 2. DDE is dichlorodiphenyldichloroethylene
- 3. DDD (TDE) is dichlorodiphenyldichloroethane
- 4. DDA is 2,2-bis(4-chlorophenyl)-acetic acid

#### What is DDT?

• DDT 1 is an organochlorine insecticide that was first synthesized in 1874 (1,2).

• DDT was a commonly-used pesticide for insect control in the United States until it was canceled in 1972 by the United States Environmental Protection Agency (EPA).

#### Why was DDT used?



• DDT was initially used by the military in WW II to control malaria, typhus, body lice, and bubonic plague . Cases of malaria fell from 400,000 in 1946 to virtually none in 1950. DDT is still used today in South America, Africa, and Asia for this purpose.

• Farmers used DDT on a variety of food crops in the United States and worldwide. DDT was also used in buildings for pest control.

• The reason why DDT was so widely used was because it is effective, relatively inexpensive to manufacture, and lasts a long time in the environment .

#### Is DDT still used?

• DDT was canceled because it persists in the environment, accumulates in fatty tissues, and can cause adverse health effects on wildlife . In addition, resistance occurs in some insects (like the house fly) who develop the ability to quickly metabolize the DDT.

#### How does DDT work?

• DDT affects the nervous system by interfering with normal nerve impulses .

#### How toxic is DDT?

#### Animals

• DDT is slightly to moderately acutely toxic to mammals, including people, if eaten.

DDT is poorly absorbed through mammalian skin, but it is easily absorbed through an insect's outer covering known as an exoskeleton .

• Laboratory animals exposed to DDT develop hyperexcitabiliy, tremors, incoordination, and convulsions

• Animals given potentially fatal doses of DDT develop liver lesions and those given DDT over a long period of time develop liver changes .

#### Humans

• People exposed to DDT while working with the chemical or by accidental exposure report a prickling sensation of the mouth, nausea, dizziness, confusion, headache, lethargy, incoordination, vomiting, fatigue, and tremors.

#### Does DDT cause reproductive or birth effects?

#### Animals

• Dogs fed DDT in low doses do not have reproductive effects.



- Rats become sterile after being fed DDT.
- Mice fed low levels of DDT have embryos that fail to attach to the uterus and irregular reproductive cycles. The offspring of mice fed DDT have a higher mortality rate.
- One of the breakdown products of DDT, DDE3, causes thinning of eggshells in birds.

#### Humans

• Scientists have no data indicating DDT causes reproductive problems or birth defects in humans.

#### **Does DDT cause cancer?**

#### Animals

• Mammals exposed to DDT develop liver tumors and have an increased risk of liver tumors .

• In one study where female and male mice consumed doses of DDT for life, the males were twice as likely to develop liver tumors .

#### Humans

• The EPA has categorized DDT as a B2 carcinogen (8). This means that DDT has been shown to cause cancer in laboratory animals, but there is inadequate or no evidence which shows that it may cause cancer in humans.

• A group of workers studied for 19 years employed at a DDT manufacturing facility did not develop cancer.

• Studies have shown that there is no correlation between an increased risk of breast cancer in women exposed to DDT (9,10,11,12,13).

#### Does DDT accumulate in humans?

#### **Fat Stores**

• DDT tends to accumulate in the fatty tissues of insects, wildlife, and people, but produces no known toxic effects while it is stored in the fat.

• DDT is metabolized into various breakdown products in the body including DDE, DDD4, and DDA5.

• When fat stores are used during periods of starvation the breakdown products of DDT are released into the blood where they may be toxic to the liver and the nervous system.

• Once DDT has accumulated in the body, it is excreted in the urine, feces, or breast milk. Breast milk is often used to measure a population's exposure to DDT.

#### Biomagnification

• Because of DDT's chemical properties it has the tendency to accumulate in animals. As animals lower on the food chain are eaten by other animals higher up, DDT becomes concentrated in the fatty tissues of predators. This continues until the primary predator of the food chain receives the highest dose, which may lead to adverse health effects. Once the use of DDT was discontinued in the U.S., its concentration in the environment and animals decreased.

#### What happens to DDT in the environment?

• DDT is highly persistent in the environment. The soil half-life for DDT is from 2 to 15 years Half-life is the time required for half of the compound to degrade.

1 half-life = 50% degraded

2 half-lives = 75% degraded

3 half-lives = 88% degraded

4 half-lives = 94% degraded

5 half-lives = 97% degraded

Remember that the amount of chemical remaining after a half-life will always depend on the amount of the chemical originally applied.

• The half-life of DDT in an aquatic environment is about 150 years

#### What effects does DDT have on wildlife?

• DDT is slightly to moderately toxic to birds when eaten. DDE decreases the reproductive rate of birds by causing eggshell thinning and embryo deaths.

• DDT is highly toxic to aquatic animals. DDT affects various systems in aquatic animals including the heart and brain.

• DDT is highly toxic to fish. Fish have a poor ability to detect DDT in water.

• DDT moderately toxic to amphibians like frogs, toads, and salamanders. Immature amphibians are more sensitive to the effects of DDT than adults.

#### PRODUCTION



Technical DDT is made by condensing chloral hydrate with chlorobenzene in concentrated sulfuric acid. It was first synthesized in 1874, but it was not until 1939 that Müller and his coworkers discovered its insecticidal properties. Production of DDT in 1971 in the United States was estimated to be 2 million kg.

This represented a sharp decline from the 82 million kg produced in 1962, and from the 56 million kg produced in 1960. At the peak of its popularity in 1962, DDT was registered for use on 334 agricultural commodities and about 85,000 tons were produced (Metcalf 1995). Production then declined and by 1971, shortly before it was banned in the United States, production had dipped to about 2,000 tons. The cumulative world production of DDT has been estimated as 2 million tons. As of January 1, 1973, all uses of DDT in the United States were canceled except emergency public health uses and a few other uses permitted on a case-by-case basis (Meister and Sine 1999). Currently, no companies in the United States manufacture DDT (Meister and Sine 1999). DDT is presently produced by companies in Mexico and China (Meister and Sine 1999). p,p'-DDD has been used as an insecticide, but is no longer produced commercially. It was prepared by condensing dichloroacetaldehyde with chlorobenzene (Budavari et al. 1996). No past production figures are available for this chemical, and there are no indications that production was ever very high. o,p'-DDD (Mitotane) is produced by Bristol, Meyer, Squibb under the brand name Lysodren® for use as a chemotherapy drug for adrenal gland cancer (PDR 1999). DDD and DDE are degradation products formed by dehydrohalogenation of DDT.

Analytical studies have shown that DDT compounds, including p,p'-DDT and p,p'-DDE, may be contaminants in technical grades of the insecticide, dicofol (Risebrough et al. 1986). In addition, another DDT-related impurity in dicofol, 1,1,1,2-tetrachloro-2,2-bis(p-chlorophenyl)ethane, has been shown to degrade to p,p'-DDE.

#### Gammexene

Lindane, also known as gamma-hexachlorocyclohexane ( $\gamma$ -HCH), gammaxene, Gammallin and sometimes incorrectly called benzene hexachloride (BHC), is an organochlorine chemical and an isomer of hexachlorocyclohexane that has been used both as an agricultural insecticide and as a pharmaceutical treatment for lice and scabies ...



IUPAC name of gammexene or benzene hexachloride (BHC) is 1,2,3,4,5,6hexachlorocyclohexane

Insecticide lindane found to cause cancer. Lindane has been banned or restricted in most countries since 2009 under the Stockholm Convention on Persistent Organic Pollutants. It was previously used extensively for insect control in agriculture and continues to be used in some developing countries.

#### GENERAL INFORMATION

Lindane belongs to the organochlorine (OC) pesticide class. This is one of the oldest classes of pesticides, and few OCs are still in use today. OC pesticides are so named because they include carbon, hydrogen, and chlorine. There are three major subclasses of OC pesticides: diphenyl aliphatics, cyclodienes, and hexachlorocyclohexane (HCH). The well-known pesticide DDT belongs to the first class. The HCH subclass is not so much a class as the collection of the five isomers of HCH: alpha ( $\alpha$ ), beta ( $\beta$ ), gamma ( $\gamma$ ), delta ( $\delta$ ), and epsilon ( $\epsilon$ ). Only the gamma isomer has insecticidal properties. This is the isomer manufactured as lindane.1 Lindane has not been produced in the United States since 1977, but it is imported in multiple forms for pharmacologic and industrial use. The use of lindane is restricted by the EPA; it can be applied only by certified pesticide applicators.

Lindane production involves the purification of technical grade HCH (16 percent  $\alpha$ -HCH, 7 percent  $\beta$ -HCH, 45 percent  $\gamma$ -HCH) to a 99.8 percent pure product. The  $\alpha$ -HCH and  $\beta$ -HCH isomers (which have a half-life of seven to eight years) are metabolized, but  $\gamma$ -HCH is metabolized much faster (its half-life is less than one day); therefore, most metabolites recovered in urine are from the gamma isomer (i.e., lindane). The most common human metabolites observed are 2,3,5-trichlorophenol, 2,4,5-trichlorophenol, 2,4,6-trichlorophenol, and 2,4-dichlorophenol (Angerer et al., 1983). Lindane has been used to control a wide variety of insect pests in agricultural, public health, and medicinal applications. It is available as a suspension, emulsifiable concentrate, fumigant, seed treatment, wettable and dustable powder, and ultra-low-volume (ULV) liquid. The chemical identity of lindane is shown in Table 4.1, and Table 4.2 summarizes its physical and chemical properties.

S.N	QUESTIONS	OPTION-A	OPTION-B	OPTION-C	OPTION-D	ANSWER
0						
1	Monochlorobenzene is	DDT	Dichloropropene	Ethylene	Trichloroethan	DDT
	reacted with hydrated			dichloride	e	
	chloral to give					
2	DDT is a	Liquid	Liquid crystals	Granular	crystalline	Crystalline solids
				solids	solids	
3	DDT can be crystallizing by	ethane	Propyl alcohol	acetone	Benzene	Propyl alcohol
4	In synthesis of DDT which	Sulphuric acid	Hydrochloric acid	Nitric acid	Acetic acid	Sulphuric acid
	is used as catalyst					
5	To remove excess acid in	Sodium	Sodium hydroxide	Potassium	Sodium	Sodium bicarbonate
	DDT is	carbonate		hydroxide	bicarbanote	
6	DDT ha a odour of	Fresh apples	Orange	Grapes	Pine apple	Fresh apples
7	The colour of DDT is	Yellow	Colourless	Pink	Brown	Colourless
8	DDT was first synthesized	1876	1872	1874	1879	1874
	in					
9	The insecticidal action of	1929	1949	1946	1939	1939
	DDT is discovered in					
10	The melting point of DDT is	109°C	106°C	108°C	105°C	108°C
11	The boiling point of DDT is	260°C	263°C	273°C	293°C	260°C
12	DDT was first synthesized	Othmar zeidler	Adolf von baeyer	Paul hermann	Monad and	Othmar zeidler
	by		-	muller	Jacob	
13	The insecticidal action of	Adolf von	Monad and Jacob	Paul hermann	Othmar	Paul hermann
	DDT is discovered by	baeyer		muller	zeidler	muller
14	The paul hermann muller	1979	1986	1989	1948	1948
	were awarded nobel prize in					
15	The DDT was banned in	1986	1979	1989	1990	1989
16	DDT was synthesised by	Addition	Elimination method	Substitution	Condensation	Condensation
		method		method	method	method
17	DDT is described as	Biopesticides	Persistent	Biodegradabl	None of these	Persistant
				e		
18	The paul hermann muller	DDT	Dichloropropene	Glyphosate	Acetic acid	DDT

	were awarded nobel prize					
19	DDI is a	Organophosph ate	Carbamate	Organochlori ne	Organosulphat e	Organochlorine
20	DDT is an	Miticides	Insecticides	Fungicides	Herbicides	Insecticides
21	Othmar zeidler is an	German chemist	Swiss chemist	Sweden chemist	Austrian chemist	Austrian chemist
22	Paul hermann muller is an	German chemist	Swiss chemist	Sweden chemist	Austrian chemist	Swiss chemist
23	DDT is used to control	Malaria	Yellow fever	Lices	Scabies	Malaria
24	Chemical formula of DDT is	C <sub>14</sub> H <sub>9</sub> Cl <sub>14</sub>	$C_{15}H_9Cl_{11}$	$C_{14}H_9Cl_{15}$	$C_{14}H_{10}Cl_{12}$	C14H9Cl15
25	Dicophane is atread name of	Dichloroprope ne	DDT	Glyphosate	Chloral	DDT
26	DDT is insoluble in	Organic solvents	Fats	Oils	Water	Water
27	DDT is soluble in	Organic solvents	water	HC1	HNO <sub>3</sub>	Organic solvents
28	Gammaxene is also called as	DDT	Lindane	Propene	Chlorobenzen e	Lindane
29	Gammaxene is an isomer of	Chlorobenzene	Hexachlorocyclohex ane	Lindane	None of these	Hexachlorocyclohex ane
30	Gammaxene is used to treat	Lice and Scabies	Scabies only	Lice only	Malaria	Lice and Scabies
31	Lindane is an	Fungicides	Insecticides	Herbicides	Miticides	Insecticides
32	Lindane is also called as	Alpha-HCH	Beta-HCH	Gamma- HCH	BHC	Gamma-HCH
33	Sometimes lindane is also called as	BHC	НСН	Gamma- HCH	Alpha-HCH	внс
34	Molecular formula for gammaxene	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	C9H9Cl9	C14H9Cl15	C <sub>6</sub> H <sub>13</sub> Cl <sub>3</sub>	C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>
35	Lindane it affect	Respiratory	Spinal cord	Nervous	Lungs	Nervous
36	Nerves, kidney and liver are	DDT	Dichloropropene	Gammaxene	None of these	Gammaxene

	affected by					
37	Lindane is an	Organophosph ate	Carbamate	Sulphonoylur ea	Organochlorin e	Organochlorine
38	Which is neurotoxic chemical	Gammaxene and DDT	DDT	Glyphosate	Carbamate	Gammaxene and DDT
39	The gammaxene was originally synthesised in 1825 by	Orthmar zielder	Faraday	Paul hermann muller	Monad and Jacob	Faraday
40	Faraday synthesised gammaxene in	1835	1823	1824	1825	1825
41	The pesticidal action of gammaxene was discovered in	1940	1942	1924	1943	1942
42	The gammaxene is almost banned in	105	100	94	96	105
43	Pharmaceutical treat for lice and scabies is	Gammaxene	DDT	Glyphosate	Carbamate	Gammaxene
44	The isomers of gammaxene is also	Production	Sales in market	Banned	None of these	Banned
45	Lindane or Gammaxene is used to treat	Third line	First line	Fourth line	Second line	Second line
46	BHC is mainly used to control	White ant	Soil pollution	Ground water	fruits	White ant
47	The boiling point of gammaxene is	325°C	323°C	321°C	329°C	323°C
48	Toxicity of gammaxene is	Natural compound	Organochlorine	Phosphate	phosphonates	Organochlorine
49	Gammaxene is also synthesised by	Monochromati c light	X-rays	UV-rays	Gamma rays	UV-rays
50	Benzene hexachloride BHC IS	Gammaxene	DDT	Glyphosate	Dichloroprope ne	Gammaxene
51	Which is polyhalogenated compound	DDT	Gammaxene	Glyphosate	Dichloroprope ne	Gammaxene

52	Gammaxene is prepared by	Substitution	Radical elimination	Condensation	Radical addition	Radical addition
53	By radical addition which compound is prepared	Glyphosate	DDT	Gammaxene	Sulphur	Gammaxene
54	The melting point of gammaxene is	112°C	113°C	111°C	110°C	112°C
55	Gammaxene is a	Solid	Liquid crystals	Crystalline	Gas	Crystalline
56	The solubility of gammaxene in water is	Soluble	Insoluble	Partially soluble	None of these	Insoluble
57	The colour of gammaxene	Yellow	White	Brown	Pink	White
58	The gammaxene is soluble in	Water	Fats	Organic solvents	Acids	Organic solvents
59	How many percentage of gammaxene is used in agricultural field	70%	80%	90%	100%	80%
60	The gammaxene is largely produced in	USA	India	China	Russia	USA
61	The molecular weight of gammaxene is	295	293	290	289	290



#### Unit IV

Synthesis and technicalmanufacture and uses of Organophosphates (Malathion, Parathion ); Carbamates (Carbofuranand carbaryl)

A discussion of the hazards to health and the environment associated with the widespread agricultural use of carbamate pesticides as insecticides, fungicides, herbicides, nematocides, and sprout inhibitors. Because of the exceptionally large number of carbamates developed and marketed over the past 40 years, the book concentrates on the analysis of selected well-known carbamates that can be used to illustrate the kinds of data available and the range of known or suspected risks. The main part is devoted to a detailed assessment of toxicity. Information includes a review of studies on the metabolism and fate of carbamate pesticides in plants, which are of particular value in the assessment of hazards to humans consuming contaminated fruits and vegetables. A discussion of effects on experimental animals and in vitro test systems summarizes what has been learned after more than two decades of short- and long-term toxicity studies. A final section concentrates on risks associated with occupational exposure in spraymen applying these insecticides

#### Chlorpyrifos General Information.

Chlorpyrifos is a broad-spectrum insecticide originally used primarily to kill mosquitoes, although it is no longer registered for this use. It is registered for a variety of uses and sites and is effective in controlling cutworms, corn root worms, cockroaches, grubs, flies, termites, fire ants, and lice.

Chlorpyrifos acts primarily as a contact poison, with some action as a systemic poison. It is available in a variety of formulations, including granules, wettable powder, dustable powder, and emulsifiable concentrate.

Environmental Characteristics of Chlorpyrifos. Due to its strong affinity for organic soils, chlorpyrifos adsorbs strongly to soils and sediments, and leaching and runoff are not significant.



Adsorbed chlorpyrifos degrades under UV light, via chemical hydrolysis, and by the action of soil microbes. The soil half-life of chlorpyrifos ranges from two weeks to more than one year, depending on soil texture, soil pH, and climate. When applied to moist soils, chlorpyrifos has a volatility half-life of 45 to 163 hours, with 62 to 89 percent of the application remaining on the soil after 36 hours (Kamrin, 1997).

#### Malathion

Malathion, also called carbophos, mercaptothion, and maldison, broad-spectrum organophosphate insecticide and acaricide (used to kill ticks and mites). Considerably less toxic to humans than parathion, malathion is suited for the control of household and garden insects and is important in the control of mosquitoes, boll weevils, fruit flies, and lice.

Malathion is a colourless to yellow-brown liquid with a characteristic unpleasant odour. It is generally prepared by combining O,O-dimethyl phosphorodithioate with diethyl maleate. It is soluble in most organic solvents except paraffin hydrocarbons and is practically insoluble in water. Malathion is readily decomposed by alkalies. The chemical works by binding to the enzyme acetylcholinesterase (AChE) at nerve endings, thus disrupting the neurotransmitter acetylcholine (ACh) and ultimately causing death.

Malathion is highly toxic to bees and other beneficial insects, aquatic invertebrates, and some species of fish, notably bluegill and largemouth bass. It is of moderate toxicity to birds.

ISO common name

malathion (E-ISO, (m)F-ISO, ESA, BAN)

Synonyms maldison, malathon, mercaptothion, mercaptotion, carbofos

Chemical names

IUPAC S-1,2-bis(ethoxycarbonyl)ethyl O,O-dimethyl phosphorodithioate

CA butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethyl ester Structural formula





MolecularformulaC<sub>10</sub>H<sub>19</sub>O<sub>6</sub>PS<sub>2</sub>

#### PRODUCTION

S-1,2-di(ethoxycarbonyl)ethyl The organophosphorus insecticide. O,O-dimethyl phosphorodithioate (common chemical name: malathion), is commercially produced in the United States and abroad. Malathion is not known to occur as a natural substance (IARC 1983). It is produced commercially by the reaction of phosphorus pentasulfide (P2S5) with methanol in toluene solvent to produce an intermediate, dimethylphosphorodithioic acid (DMPDT), and a byproduct, hydrogen sulfide (H2S) (Sittig 1980). The DMPDT intermediate is isolated and then reacted with either diethylfumarate or diethylmaleate. The crude material is then stripped of solvent, washed, and filtered to produce technical-grade malathion. Malathion was first commercially produced in the United States in 1950 by American Cyanamid Chemical Company (USTC 1953) and was first registered in the United States in 1956. Manufacturing rights were transferred to Cheminova Agro, Inc. in 1991 (EPA 1999). Production volume data were not located for the 1950s and 1960s. The production of malathion was estimated to be 24 million pounds in 1972 (Santodonato 1985; von Rumker et al. 1974) and 30 million pounds in 1978 (IARC 1983). No recent production volume data are available for malathion.

#### **Methods of Manufacture**



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Malathion is typically manufactured using a condensation reaction (at 70-80 °C) of O,Odimethyl phosphorodithioic acid and diethyl maleate or diethyl fumarate in the presence of hydroquinone.

The feed materials for malathion manufacture are O,O-dimethyl phosphorodithioic acid and diethyl maleate or fumarate. ... An antipolymerization agent such as hydroquinone may be added to the reaction mixture to inhibit polymerization of the maleate or fumarate compound under reaction conditions. This reaction is preferably carried out at temperatures within the range of 20 deg to 150 °C. This reaction is preferably carried out at atmospheric pressure. ... The reaction is preferably carried out in a solvent such as the low molecular weight aliphatic monohydric alcohols, ketones, aliphatic esters, aromatic hydrocarbons or trialkyl phosphates. ... A stirred, jacketed reactor of conventional design may be used. After cooling, the reaction mixture may be taken up in benzene. It is then washed with 10% Na2CO3 and with water. The organic layer is dried over anhydrous Na2SO4, filtered and concentrated in vacuo to give the final product as residue.

Technical grade malathion may contain malaoxon, isomalathion, or other organophosphates as impurities. These compounds inactivate carboxylesterases, thus increasing malathion toxicity by decreasing the hydrolysis of the drug and increasing the amount of the drug that is oxidized to malaoxon.

The analysis of technical organophosphorus insecticides by (31)P nuclear magnetic resonance showed the major known toxic contaminants to be simple trialkyl phosphorothio- and -dithioic acid esters and the S-alkyl insecticide isomers. Small amt of the bis derivatives and the dithiopyrophosphate were also detected. These contaminants included both byproducts from the synthesis as well as degradation products. This procedure was used to analyze the following technical grade products: ronnel, sulfotepp, methyl parathion, dimethoate, malathion, methidathion, ethion, phosalone, and fenitrothion.

#### Synthesis of malathion



Malathion is produced by the addition of dimethyl dithiophosphoric acid to diethyl maleate or diethyl fumarate. The compound is chiral but is used as a racemate.



Uses:

- Malathion is a broad-spectrum insecticide used to control a variety of outdoor insects in both agricultural and residential settings. Malathion is registered for use on food, feed, and ornamental crops and in mosquito, boll weevil and fruit fly eradication programs.<sup>1</sup> Uses for individual malathion products vary widely. Always read and follow the label when applying pesticide products.
- Malathion is also an ingredient in shampoos regulated by the United States Food and Drug Administration (FDA) to control head lice.<sup>1</sup>
- Signal words for products containing malathion may range from Caution to Danger. The signal word reflects the combined toxicity of the active ingredient and other ingredients in the product.

#### Synthesis and technical manufacture Parathion

**Parathion** is **synthesized** from diethyl dithiophosphoric acid  $(C_2H_5O)_2PS_2H$  by chlorination to generate diethylthiophosphoryl chloride  $((C_2H_5O)_2P(S)Cl)$ , and then the chloride is treated with sodium 4-nitrophenolate (the sodium salt of 4-nitrophenol).

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#### **Technical manufacture of Parathion**

In the 1st step, ethyl dithiophiosphone acid ... /is/ prepared by reacting ... anhydrous ethyl alcohol with ... phosphorous pentasulfide. ... The chlorination step follows & may use elemental chlorine, sulfur monochloride or sulfur dichloride. ... A production & waste schematic for the overall process of parathion manufacture /for a typical plant producing 20,000 tons per year/ is. ... /described by/ Gruber GI (TRW Systems Group); Report EPA/530/SW-118c, Washington, DC, USEPA (April 1975). To ... thiophosphoryl chloride ... an approx 20% soln of sodium ethylate in ethyl alcohol /is added/. ... To this mixture ... p-nitrophenol ... /was added/ & to this resulting solution was added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol was added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol /is added. ... Approx 20% soln of sodium ethylate in ethyl alcohol ... water /is added to the reaction mixture/ in order to dissolve sodium chloride & to separate the O,O-diethyl O-p-nitrophenyl thiophosphate from the residual alcohol.

The following impurities were identified in one sample of technical-grade parathion: O,O-diethyl thiophosphoryl chloride; O,O,O-triethyl thiophosphate; O,O-diethyl S-ethyl thiophosphate; O,O-



diethyl S-ethyl dithiophosphate; nitrophenetole; nitrophenol; parathion isomers; & the dithio analogue of parathion.

The analysis of technical organophosphorus insecticides by (31)P nuclear magnetic resonance showed the major known toxic contaminants to be simple trialkyl phosphorothio- and -dithioic acid esters and the S-alkyl insecticide isomers. Small amt of the bis derivatives & the dithiopyrophosphate were also detected. These contaminants included both byproducts from the synthesis as well as degradation products. This procedure was used to analyze the following technical grade products: ronnel, sulfotepp, methyl parathion, dimethoate, malathion, methidathion, ethion, phosalone, & fenitrothion. /Organophosphorous insecticides/

#### Uses

Parathion controls a variety of insects such as aphids, mites, beetles, Lepidoptera, leaf hoppers, leafminers, and other pests found on fruits, cotton, vegetables, and forage crops. It also controls several soil insects such as wireworms, rootworms, and symphilids.

Used for control of nematodes in beet & ornamentals



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Non-systemic insecticide and acaricide; used for the control of sucking and chewing insects (including soil insects) and mites in a very wide range of crops.

S	QUESTIONS (Unit-IV)	OPTION-A	OPTION-B	OPTION-C	OPTION-D	ANSWER
Ν						
0	Which is as arganaphasphata	Commoyona		Malathian	Carbofuron	Molothion
1		Gammaxene		Malatinon	Carbonuran	
2	Organophosphate is an	Insecticides	Herbicides	Fungicides	Miticides	Insecticides
3	In USSR malathion is also called	Carbophos	Maldison	Mercapthion	Glutamate	Carbophos
	as	_		_		-
4	The appearance of the malathion is	Solid	Liquid	Gas	Crystalline	Liquid
5	To eradicate mosquitoes which is used	Malathion	Gammaxene	DDT	Glyphosate	Malathion
6	The melting point of malathion is	276	278	279	226	276
7	The boiling point of the malathion is	429	426	414	417	429
8	Anatoxin-a(s) is a naturally occuring organophosphate	Viruses	Cynobacteria	Lactobacteria	Fungi	Cynobacteria
9	Malathion is acts as an	Acetylnitroest er	Acetylfluroester	Acetylcholinest er	Acetylchloroest er	Acetylcholineste r
10	Malathion is also known as	Carbophos	Acetylcholinest er	Maldison	Mercapthion	Acetylcholineste r
11	The smell of malathion is	Fruity odour	Fisher odour	Rotten egg smell	Garlic smell	Garlic smell
12	The over dosage of malathion can causes	Blood cancer	Liver cancer	Lung cancer	Pancreas cancer	Liver cancer
13	The molecular weight of the malathion is	330	337	336	365	330
14	The impure colour of the malathion is	Red	Yellow	Blue	Green	Yellow
15	Most of the impurities in malathion percentage of	90	91	85	99	90
16	The density of the malathion is	1.23	1.24	1.26	1.21	1.23

17	The malathion is well soluble in	Ethanol	Acetone	Benzene	Ethyl ether	Ethyl ether
18	Malathion is prepared by	Subsitution	Addition	Elimination	Condensation	Addition
19	The nature of the malathion is	Acid	Base	Salt	Neutral	Acid
20	The malathion is	Symentry	Asymentry	Chiral	Achiral	Chiral
21	Malthion is also an ingredient in	Soap	Shampoo	Face cream	Talcum powder	Shampoo
22	In malathion the source of carbon and phosphorous are	Viruses	Fungi	Bacteria	Mildew	Bacteria
23	Malaoxone is consides as an how many times more toxic than malathion	22	11	33	26	22
24	The malathion is degrade by	Nitroxy ester	Carboxy ester	Methoxy ester	Hydroxy ester	Carboxy ester
25	The vapour pressure of the malathion is	1.2	1.4	1.3	1.6	1.2
26	The malathion is the	Natural	synthatic	biopesticides	Fungicides	Synthatic
27	Malathion is a compound of	Pt	Cl	0	Р	Р
28	For the treatment of pediculosis capitis	Gammaxene	Malathion	Parathion	Carbofuran	Malathion
29	The parathion is an	Acaricides	Miticides	Herbicides	Rotendicides	Acaricides
30	Parathion is an	Brown crystal	Black crystal	White crystal	Yellow crystal	White crystal
31	The trade name of carbofuran is	Chlorodan	Iodiane	Furadan	Cholin	Furadan
32	The most toxic carbamate pesticides is	Carbofuran	Parathion	Carbaryl	Malathion	Carbofuran
33	The carbofuran is the	Biopesticides	synthetic	Natural	Herbicides	Synthetic
34	The carfuran is banned in	USSR	Spain	Nepal	Canada	Canada
35	Carbofuran is particullarly toxic to	Animals	Rotends	Mites	Birds	Birds

36	The appearance of the carbofuran is	Crystalline	Solid	Liquid	Gas	Solid
37	The carbofuran has an	Garlic	Odourless	Pine apple	Onion	Odourless
38	Hydrogen bond donar count in a carbofuran is	1	2	3	4	1
39	Hydrogen bond acceptor count in the carbofuran is	3	4	5	6	3
40	The melting point of the carbofuran has	151	141	121	131	151
41	The boiling point of the carbofuran is	313	414	323	333	313
42	The brand name of the carbaryl is	Bayer	Furadan	Sevin	Carbide	Sevin
43	The carbaryl is prepared by	Addition	Elimination	Condensation	Direct method	Direct method
44	The carcinogenic causing pesticides is	Carbofuran	Malathion	Parathion	Carbaryl	Carbaryl
45	The carbaryl is introduced commercially in the year of	1958	1964	1982	1996	1958
46	Which of the following is known as veterinary drug	Parathion	Carboxy ester	Carbaryl	Carbofuran	Carbaryl
47	The density of the carbaryl is	1.2	1.3	1.4	1.5	1.2
48	The carbaryl is insoluble in	Ethanol	Ether	Benzene	Water	Water
49	The molecular weight of the carbaryl is	201	202	203	204	201
50	Hydrogen bond count in carbaryl is	1	2	3	4	1
51	Hydrogen bond acceptor count in the carbaryl is	2	3	4	1	2

52	The carbaryl has an	Garlic	Pine apple	Odourless	Orange	Odourless
53	The melting point of the carbaryl	142	132	153	165	142
	is					
54	The boiling point of the carbaryl is	Decomposes	150	132	154	Decompose
55	The carbaryl has been used for	30 years	32 years	54 years	65 years	30 years
	about					
56	Aphids, fire, ants, fleas are killed	Malthiom	Carboxy ester	Carbaryl	Carbofuran	Carbaryl
	by					
57	190 register pesticides products	Carbofuran	Carbaryl	Malathion	Parathion	Carbaryl
	that contain					
58	The converted to carbaryl by the	Amine	Amide	Ammonia	Methyl amine	Methyl amine
	reaction with					
59	Carylderm shampoo used to	Head lice	Skin	Leg lice	Lice	Head lice
	combat					
60	The veterinary drug carbaril is	Carbofuran	Malathion	Parathion	Carbaryl	Carbaryl



#### Unit V

Synthesis and technicalmanufacture and uses of Quinones ( Chloranil), Anilides (Alachlor and Butachlor).

Chloranil is aeromatic organic compound synthesized from hydroquinone which is used as intermediate in dyes and pigments, diaziquone (azq), a cancer chemotherapeutic agent. Use as aromatization for synthesis of carpofren.



A 2-liter three-necked flask is fitted with an airtight stirrer, gas inlet tube, and reflux condenser. In the flask are placed 47 grams (0.5 mole) of phenol, or 65 grams of orto or pchlorophenol, and 1 liter of concentrated hydrochloric acid. Stirring is started, sufficiently vigorously to break up the mixture into very fine droplets, and a rather rapid stream of gaseous chlorine is introduced. The gaseous chlorine need not be specially dried, but it should be run through a wash bottle of sulfuric acid to show the velocity of the gas stream. The temperature rises to about 40°C. After 4 hours, the reaction flask is surrounded by a 70° water bath, and the introduction of gaseous chlorine is continued until the obtained solution is completely saturated, requiring about 20 hours. As the chlorination proceeds, some crystals form on the upper part of the flask and in the condenser. When no more gaseous chlorine is being absorbed, the gas introduction tube is replaced by a dropping funnel, and 250 ml. conc. nitric acid is added over a period of 3 hours, while stirring is continued and the temperature is held at 80-85°. At first, a vigorous reaction takes place, but this soon subsides. The reaction



mixture becomes red and the crystals dissolve. After the nitric acid has all been added, stirring is continued for 20 hours at a temperature of 85°. Heavy, plate-like, yellow crystals separate gradually. These are filtered off, after cooling, and washed first with 2 liters of water, then with 250 ml. alcohol to remove a reddish oily impurity. The product is then dried at 80°. The obtained product melts at 285-286° and is practically pure chloranil. The yield is 70 to 75 grams, or almost 60 % of the theoretical amount. Remarks. All chloro derivatives of phenol are converted to chloranil by the above procedure.



24 g of 2,6-dichlor-4-nitraniline are reduced to the corresponding diamine by boiling with 600 ml of concentrated hydrochloric acid and 26 g of metallic tin. Without cooling, 20 g of crystallised potassium chlorate are slowly added, the whole being kept gently boiling. The boiling is continued for a few minutes after the whole of the potassium chlorate has been added, and the liquid then diluted and filtered. The precipitate is well washed with water, dried, and then purified either by recrystallisation from toluene or by sublimation. Yellow leaflets which sublime on heating. Yield 90%.



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**UNIT-V** 

#### Uses:

CHLORANIL (2,3,5,6-TETRACHLORO-P-BENZOQUINONE) Chloranil is used as a fungicide.

It is used as an oxidizing agent in the organic synthesis especially for dye intermediates and vulcanization agent.

Benzoquinone is used as an oxidizing agent in organic synthesis.

#### Alachlor

Alachlor is an aniline herbicide used to control annual grasses and certain broadleaf weeds in field corn, soybeans and peanuts. It is a selective systemic herbicide, absorbed by germinating shoots and by roots. The compound works by interfering with a plants ability to produce (synthesize) protein and by interfering with root elongation

#### **Common name Alachlor**

Chemical name and other names or synonyms IUPAC:

2-chloro-2',6'-diethyl-N-methoxymethylacetanilide

2-chloro-N-(2,6-diethylphenyl)-N-(methoxymethyl)acetamide

Trade names: Alanex, Bronco, Cannon, Crop Star, Lasso, Lariat, Partner, Reneur, Traton



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#### Molecular formula C14H20ClNO2

Chemical structure

Reaction of chloroacetyl chloride with azomethine or 2,6-diethylaniline and formaldehyde, followed by treatment with methanol.

#### Synthesis and technical manufacture and uses Butachlor

Butachlor is an herbicide of the acetanilide class. It is used as a selective pre-emergent herbicide.

An analytical method using a macroporous diatomaceous earth column and florisil cartridge for cleanup procedure was developed for determination of butachlor and pencycuron in vegetables and rice.

Butachlor is the most commonly used herbicide on paddy fields in Taiwan and throughout Southeast Asia.





Butachlor-degrading bacteria were isolated using enrichment culture technique.

The solid-phase microextraction technique using a 100  $\mu$ m film poly(dimethylsiloxane) has been examined with the aim to determine butachlor in aqueous samples.

Butachlor can be Used pre-emergence for the control of annual grasses and certain broad-leaved weeds in rice, both seeded and transplanted. It shows selectivity in barley, cotton, peanuts, sugar beet, wheat and several brassica crops.

Butachlor and pyrazosulfuron-ethyl are two new highly active herbicides that have been extensively used to control a wide range of weeds in a variety of vegetables and other crops.

Degradation of the herbicide butachlor was investigated using laboratory-synthesized zerovalent iron . The synthesized zerovalent iron was determined to be nanoscale powder by scanning electron microscopic analysis.

China's butachlor capacity is 6 000 t/a today and output is around 4 000 tons a year.

The market price of 50% butachlor emulsion oil was RMB28 000 per ton in the brisk application season, being 19% higher than that in the same period of last year.



Butachlor domestic production capacity of 6,000 tons / year, the actual output of about 4,000 tons / year, domestic consumption of 3,000 tons / year, exports of 1,000 tons / year in recent years the market showed a saddle-type development. 2007,2008 national rice procurement price is too low for two years, the enthusiasm of farmers to plant rice decreased significantly cut paddy field area, and to plant corn, soybeans and other dry land crops, the use of butachlor has dropped significantly.



#### Application

Bio-efficacy of Pre and Post-emergence Herbicides in Transplanted Aromatic Basmati Rice Determination of Butachlor and Pencycuron Residues in Vegetables and Rice: Application of the Macroporous Diatomaceous Earth Column

Histopathological study on the effect of rice herbicides on grass carp (Ctenopharyngodan idella) Effects of the herbicide, Butachlor on nitrogen fixation in phototrophic nonsulphur bacteria. The phylogenic changes in diazotrophic population under butachlor application in paddy soil **Properties** 

Assessment of genotoxic effects of Butachlor in fresh water fish, Cirrhinus mrigala(Hamilton)

Effect of Butachlor Herbicide on Earthworm Eisenia fetida-Its Histological Perspicuity



Summary of Toxicology Studies with Butachlor

Toxicity studies of butachlor to the freshwater fish Channa punctata (Bloch)

A water-soluble inclusion complex for butachlor was prepared by complexation with (2-hydroxypropyl)- $\beta$ -cyclodextrin (HP- $\beta$ -CD). Phase solubility results indicated a 1:1 stoichiometric ratio with an apparent stability constant of 864.3 M–1 in the obtained solid complex

#### **Application of Chloranil :**

Benzoquinone is used in organic chemistry as an oxidizing agent. Strongly oxidizing quinones include chloranil and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (also known as DDQ).

Chloranil is used as a fungicide. It is used as an oxidizing agent in the organic synthesis especially for dye intermediates and vulcanization agent.

Benzoquinone is used as an oxidizing agent in organic synthesis. Some substituted benzoquinones are stronger reagents e.g o-chloranil, p-chloranilexist (tetrachlorobenzoquinone), and DDQ (2,3-dicyano-5,6-dichloro-parabenzoquinone). They are used as reagents for the oxidation (including oxidative coupling and cyclization reaction) and dehydrogenation of hydroaromatic compounds. They are useful in the synthesis of aromatized or lactones formed steroids and modified natural products. Metal dioxide such as selenium dioxide and manganese dioxide are also oxidising agents which convert alcohols into ketones, aromatic methyl groups into aldehyde or carboxylic acids, double bonds into alcohols, aldehydes into carboxylic acids, steroidal ketones into secolactones. But several side reactions are expected due to the lack of selectivity. DDQ and substituted quinones provide regioselective effectiveness for the



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preparation of target intermediates. Phenylbis(trifluoroacetato-O)iodine and Tritylium tetrafluoroborate are also reagent for the dehydrogenation of hydroaromatic compounds.



#### Unit-V

S	QUESTIONS	OPTION-A	OPTION-B	OPTION-C	OPTION-D	ANSWER
No						
1	The colour of chloranil is	Green	Yellow	Black	Orange	Yellow
2	The appearance of the chloranil is	Liquid	Crystalline	Solid	Gas	solid
3	The chloranil is an	Reducing agent	Oxidising agent	Mild	Mild	Mild oxidising
				reducing	oxidising	
4	The molecular structure of the chloranil is	Trigonal	Pyramidal	Planer	Octahedral	Planer
5	The melting point of the chloranil is	568	567	565	580	568
6	The chloranil is used to test for finding	Primary amines	Amides	Ammonia	Secondary	Secondary
		_			amines	amines
7	To check the presence of the proline	Chloranil	Alachlor	Ammonia	Amides	Chloranil
	derivatives which is used					
8	The secondary amines reacts with chloranil to	Yellow	Blue	Red	Black	Red
	give					
9	Chloranil is produced by the chlorination of	Benzene	Furan	Phenol	Thiazol	Phenol
10	Among which is used to convert	Phenol	chloranil	Alachlor	Furan	Chloranil
	cyclohexadienesto the benzene derivatives					
11	Hydrolysis of dichloromethylene group in this	Benzene	Phenol	Thiazol	Chloranil	Chloranil
	dienone gives					
12	Chloranil is more electrophilic than	Phenol	Benzene	Thiazol	Quinone	Quinone
13	The molecular mass of the chloranil is	246	247	242	226	246
14	The chloranil s serve as	H-Donar	Acid	Base	H-Acceptor	H-Acceptor
15	Which one is displace chlorides from the ring	Amide	Amines	Alachlor	Oxygen	Amide
	of quinone					
16	All chloro derivatives of phenol are convered	Quinone	Iso quinone	Chloranil	Amides	Chloranil
	to					
17	The hydrogen bond donar count in the	0	1	2	3	0
	chloranil is					

18	The hydrogen bond acceptor count in the	2	3	4	1	2
	chloranil is					
19	Chloranil is very soluble in the	Water	Ether	Alcohol	Chloroform	Ether
20	Chloranil is slowly decomposed by	Acid	Base	Alkali	Sunlight	Sunlight
21	Alachlor is an	Rotendicides	Insecticides	Miticides	Herbicides	Herbicides
22	Alachlor has an	onion odour	Garlic odour	Orange	Odourless	Odourless
23	The appearance of the alachlor is	White liquid	Yellow solid	Yellow liquid	White solid	White solid
24	The chloroacetanilide family is	DDT	chloranil	Alachlor	Malathion	Alachlor
25	Alachlor is insoluble in the	Acetone	Alcohol	Chloroform	Water	Water
26	The melting point of the alachlor is	312	313	314	315	312
27	The boiling point of the alachlor	404	405	407	420	404
28	The trade name of the alachlor is	Furadan	Sevin	Bayer	Alanex	Alanex
29	Alachlor is an	Natural	Synthatic	Insecticides	Herbicides	Herbicides
30	In alachlor how many percentage of active ingrediants are present	15	26	14	17	15
31	Alachlor can be used as the subsitution for	Nitrogen gas	Carbondioxide gas	Hydrogen gas	Methane gas	Methane gas
32	Alachlor is sparlingly soluble in the	Acetone	Chloroform	Water	Heptane	Heptane
33	In alachlor ESP is used to analysis for	Sulphur	Anilic acid	Chlorine	Oxanilic	Oxanilic
34	The hydrogen bond count in the alachlor is	0	3	2	4	0
35	The hydrogen bond acceptor count in the alachlor is	2	3	5	6	2
36	Alachlor is soluble in the	Heptane	Water	Phenol	Acetone	Acetone
37	Alachlor is used to kills	Fungi	Bacteria	Mice	Weeds	Weeds
38	The molecular weight of the alachlor is a	269	226	237	299	269
39	Alachlor can causes	Lungs	Nerves	Kidney	Heart	Kidney
40	The sorption of the alachlor in the soil is	43-209	44-209	43-210	44-210	43-209
41	Butachlor is a	Fungicides	Insecticides	Miticides	Herbicides	Herbicides

42	The herbicide of the acetanilide class is	DDT	Carbaryl	Chloranil	Butachlor	Butachlor
43	The molar mass of the butachlor is	311	312	313	326	311
44	The appearance of the butachlor is	Solid	Liquid	Gas	Oil	Oil
45	The colour of the butachlor is a	Red	Blue	Green	Yellow	Yellow
46	The odour of the butachlor is	Garlic	Fruity	Odourless	Sweet	Sweet
47	The boiling point of the butachlor is	156	132	154	158	156
48	The butachlor is soluble in the	Heptane	Ether	Phenol	Water	Ether
49	The butachlor is decomposes at	165	166	176	173	165
50	When decomposition of the butalchlor it emits	Oxides	Nitrous oxides	Chlorides	Nitrogen gas	Nitrous oxides
51	The butachlor corrodes	Aluminium	Stainless steel	Iron	Steel	Steel
52	Butachlor is stable to	Sodium light	Mercury light	UV light	Sunlight	UV light
53	The hydrogen bond donar count in the	0	2	3	6	0
	butachlor					
54	The hydrogen bond acceptor count in the	2	4	6	8	2
	butachlor is					
55	Butachlor is increase the risk in humans by	Lungs	Nerves	Eye	Neoplasms	Neoplasms
56	Butachlor is used to kill	Fungi	Bacteria	Weeds	Mice	Weeds
57	The density of the butachlor is	1.06	1.55	1	1.06	1.06
58	Butachlor is mostly used in the field of	Corn	Paddy	Wheet	Flower	Paddy
59	Among the following which is aromatic	Chloranil	DDT	Carbaryl	Butachlor	Butachlor
	amide					
60	Butachlor is also known as	Organophosphate	Organochlorine	Carbamate	DDT	Organochlorine

[18CHU402]

#### KARPAGAM ACADEMY OF HIGHER EDUCATION (Deemed to beUniversity Established Under Section 3 of UGC Act 1956) UG DEGREE EXAMINATION, DECEMBER 2019 (For the candidates admitted from 2018 onwards)

#### DEPARTMENT OF CHEMISTRY EVEN SEMESTER

#### *II B.Sc., CHEMISTRY* INTERNAL EXAM-I PHYSICAL CHEMISTRY-IV (Electrochemistry)

Time: 2 hours Date :

#### Maximum: 50 marks

#### **<u>PART- A</u>** Answer All the Questions

 $(20 \times 1=20 \text{ Marks})$ 

1.Fraction of the total a. transport number	current carried by pot b. hittorf's method	assium ion in KCl is c c. kohlrauschs law	alled d.wien effect				
2. The drag on the cen a. assymmetry effect	tral ion is known as b. symmetry effect	c. viscous effect	d.interionic eff	fect			
3. The speed of the ior a.ionic mobility	n per unit potential grad b.ionic conductance	dient is called as c.Potetial d.Cone	luctance				
4.What is the unit of λm (Molar conductance) a.Smmol-1 b.Sm mol-2 c.Sm2mol-2 d.Sm2mol-1							
5.An electrolytes Infina. $\lambda^{\circ}m$ b.1/ $\lambda^{\circ}m$	nite dilution is denoted $c.\lambda^{\circ}c  d.1/\lambda^{\circ}c$	l by					
6.Conjugate acid-base a.Strong b.weak	e pairs, if the acid is str c.neutral d.mode	rong, then base is erate					
7.The hydronium ion a.H+ b.OH- c.H3O	is represented as + d.H2O						
8.The reciprocal of re a.molar conductance	sistivity is known as b.specific conductanc	e c.equivalent c	onductance	d.permittivity			
9.Molar conductance ionisation but to fall i	decreses with increase n mobilities of ions du	in concentration is not e to greater	t due to fall the	degree of			

a.interionic effect b.wien effect c.viscous effect d.

10.Which method is used for determination of transport number?a.Hirttorf's methodb.moving boundary methodc.Debye methodd.Hirttorf's method and moving boundary method
11.Calculate the transport number of Li+ and Br- ions when a current flows through an infinitely dilute aqueous solution of LiBr at 25°c, given the ionic mobilities of Li+ and Br- ion at infinite dilution are 4.01 x 10-8 and 8.09 x 10-8 m2v-1s-1 respectively. a.0.669 b.0.996 c.0.756 d.0.825
12. Acetic acid is a weak acid, because a.it has very low tendency to donate OH- b.it has very low tendency to donate H+ c.it has very high tendency to donate H+ d.it has very high tendency to donate OH-
13. Dissociation of phosphoric acid occurs in a.three stages b.two stages c.one stages d.ten stages
14. The dissociation constant of water is a.ionic product of water b.surface tension c.viscosity d.concentration
14. According to Lowry- bronsted theory, an acid is a.donates proton b.accepts proton c.donates electron d.accepts proton
15. When acetic acid is dissolved in water, the water behaves as a.solvent b.acid c.amphoteric d.neutral
16. buffer mixture is a a.strong acid & its salt b.weak base & its salt c.weak acid & its saltd.strong base& its sal
<ul> <li>17. The equilibrium constant K is called</li> <li>a.dissociation constant of the weak electrolyte</li> <li>b.dissociation constant of the acid</li> <li>c.dissociation constant of the base</li> <li>d.dissociation constant of the electrolyte</li> </ul>
18. According to Kohlrausch's law, conductivity of ions is constant at a.fixed temperature b.infinite dilution c.1 M concentration d.all the concentrations
19. What is the unit of k (kappa) a.sm-1 b.s2m2c.s-1m d.s/m2

20. According to Kohlrausch's law, conductivity of ions at infinite dilutions does not depend on a.nature of co-ions b.temperature c.pressure d.concentration

21. The degree of dissociation of a weak electrolyte at any dilution can be calculated by the relationship of  $a.\alpha=1$   $b.\alpha=\Delta^{\circ}m/\Delta m$   $c.\alpha=-1$   $d.\alpha=\Delta m/\Delta^{\circ}m$ 

#### **PART- B (3 x 2=6 Marks)**

#### **Answer All the Questions**

21. What is meant by ionic mobilities?

22. Define Debye Falkenhagen effect?

23. What is the equivalent weight of calcium hydroxide (Ca(OH)<sub>2</sub>) and phosphoric acid (H<sub>3</sub>PO<sub>4</sub>)

? The molar mass is 74.1 and 98 g/mol.

#### PART- C (3 x 8=24 Marks)

#### **Answer All the Questions**

24. (a). Explain the Faraday's first law of electrolysis.

(**OR**)

(b) (a) Define the following terms

- (i) Electrolysis (ii) Specific conductance.
- (iii) One Faraday (ivWein Effect
- 25. (a) Explain Arrhenius theory of electrolytic dissociation

#### (**OR**)

- (b) Specific conductivity of a saturated solution of Agcl at 25°C was found to be 3.41 \* 10<sup>-5</sup> ohm<sup>-1</sup> cm<sup>-2</sup>. The specific conductivity for water used to make up the solution was 1.6\* 10<sup>-6</sup> ohm<sup>-1</sup> cm<sup>-2</sup>. Determine the solubility of AgCl in water. Ionic conductances of Ag<sup>+</sup> and Cl<sup>-</sup> at 25°C are 60.3 and 78.3 ohm<sup>-1</sup> cm<sup>2</sup> respectively.
- 26. (a) Calculate the transport numbers of Li<sup>+</sup> and Br<sup>-</sup> ions when current flows through an infinitely dilute aqueous solution of LiBr at 25<sup>o</sup>C, given the ionic mobilities at Li<sup>+</sup> and Br<sup>-</sup> ions at infinite dilution are 4.01\*10<sup>-8</sup> and 8.09\*10<sup>-8</sup> m<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>, respectively

#### (OR)

(b) How to determine the transference number using Hittorf method.

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Date : Time: 2 hours 3. 2. 2odo (AN)

a.positive

c. s <sup>-1</sup> d. mol $L^{-1} s^{-1}$	a. L mol <sup>-1</sup> s <sup>-1</sup> b. L <sup>2</sup> mol <sup>-2</sup> s <sup>-1</sup>
ion is b. directly proportional to the initial concentration d. directly proportional to the concentration	<ol> <li>Half-life period of a second order react</li> <li>independent of the concentration</li> <li>inversely proportional to concentration</li> </ol>
b.high concentration d.very low temperature	<ol> <li>When Solubility product is constant at</li> <li>very high temperature</li> <li>particular room temperature</li> </ol>
b.weak base & its salt d.strong base& its salt	<ol> <li>A buffer mixture is a a.strong acid &amp; its salt</li> <li>weak acid &amp; its salt</li> </ol>
d. a constant	<ol> <li>The value of buffer index is always</li> <li>positive b.negative c.zero</li> </ol>
d.3,4	3. The PH value of HCl and NaOH are a.1,14 b.1,1 c.14,14
OH d.H <sup>+</sup> or OH	LH <sup>+</sup> b.OH c.H <sup>+</sup> and
nsion c.viscosity d.concentration	The dissociation constant of water is ionic product of water b.surface te
RT-A the Questions (20 × 1=20 Mar	ate: 3. 2. dodo (AN) PA Answer All
Maximum: 50 Marks	
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9. Parallel reactions take place in a. more than one step

c. in one way but more than one step

d. in one step but more than one b. more than one way

ġ, a. energy of activation differs from one reaction to another 10. The rate of chemical reaction depends on the nature of chem some are solid at room temperature

0 some are coloured

d. some are solid at high temperature

a. second order reaction c: zero order reaction 11. Decomposition of nitrogen pentoxide in CCl<sub>4</sub> is an example d. first order reaction. b. third order reaction

c. second order reaction a 12. Hydrolysis of an ester by dilute HCl is an example for zero order reaction b.first order reaction

d. pseudo first order reaction

a. molecularity 13. The sum of the powers of the concentration terms that occur in the b. order c. rate d. rate constant

a.dr/dt 14 The unit for the rate is mathematically expressed as b.dp/dt

a. decrease in the concentration of a reactant 15. Rate of reation is defined as c.dc/dt d.drp/dt

Ģ 9 change in the concentration of any one of the reactants or products increase in the concentration of a product

d increase in the concentration of a reactant

a. high 16 If the activation energy is high then the rate of the reaction is b. moderate c.low d. cannot be

reaction is the 17. The minimum amount of energy required to overcome the er

a, heat of reaction.

c. KE of the reactants

B. activation energy

A reaction involving two different reactants can never be a

d. enthalpy of the products

Ģ

18

a. bimolecular reaction c. first order reaction

d. second order reaction Unimolecular reaction

a. reaction and concentration 19. Order of reaction can be identified by plotting graphs of b. concentration c.pH v

00

p

6



20. The conjugate pair of ammonia in aqueous solution is a.CH<sub>3</sub>COOH<sup>+</sup> b.NH<sub>4</sub>OH c.NH4<sup>+</sup>

 $d.H_3O^+$ 

# PART – B Answer all the Questions

(3 X 2 = 6 Marks)

21. What is meant by ionic product of water?22. Give the example of second order reaction.?23. Define hydrolysis?

# PART – C Answer all the questions

## $(3 \times 8 = 24 \text{ Marks})$

24. a) Draw and explain the titration curves obtained in conductometric titration ?
 (OR)
 b) Write a note on solubility and solubility product of sparingly soluble salts?

25. a) Derive the first order differential and integrated rate equation?
 (OR)
 b) Define chain reactions. Explain chain reaction by taking any one example?

 26. a) Explain the kinetics of opposing reactions? (OR)
 b) Explain consecutive reactions using steady sate approximation theory?

