JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

SYNTHESIS AND CHARACTERISATION OF ORGANOPHOSPHATE ESTERS

[1]Dr. Asha Verma, [2]Sheetal Meena ,[3]Bhavna Jhod

[1]Dr. Asha Verma Professor
Department of Chemistry, Govt. Dr. Shyama Prasad Mukherjee Science and Commerce College Kolar, Bhopal (Madhya pradesh),

[2]Research Scholar Department of Chemistry, Govt. Dr. Shyama Prasad Mukherjee Science and Commerce College Kolar ,Bhopal (Madhya Pradesh),

[3]Bhavna jhod Research Scholar Department of Chemistry, Govt. Dr. Shyama Prasad Mukherjee Science and Commerce College Kolar ,Bhopal (Madhya Pradesh).

***Abstract*:** An organophosphate refers to the ester of phosphoric acid. Phosphates are most probably the most prevalent organo phosphorus compounds. The chemistry of phosphate esters continues to draw the attention of chemists due to their versatile applications in the analytical, biological, and industrial fields. The most important organo-phosphorus compounds are phosphate esters which are based on P-O-C linkages. Phosphorus chemistry is dominated by oxy phosphorus compounds, all of which contain phosphorus-oxygen linkage Most of these are usually known as phosphates.

***Key Words*: -** organophosphate, versatile, linkage.

I. INTRODUCTION

In organic chemistry, organophosphates (also known as phosphate esters, or OPEs) are a class of organophosphorus compounds with the general structure $O{=}P(OR)_3$, a central phosphate molecule with alkyl or aromatic substituents.[1] They can be considered as esters of phosphoric acid. Organophosphates are best known for their use as pesticides. Like most functional groups, organophosphates occur in a diverse range of forms,[2] with important examples including key biomolecules such as DNA, RNA and ATP, as well as many insecticides, herbicides, nerve agents and flame retardants.

OPEs have been widely used in various products as flame retardants, plasticizers, and performance additives to engine oil. The low cost of production and compatibility to diverse polymers made OPEs to be widely used in industry including textile, furniture, electronics as plasticizers and flame retardants. These compounds are added to the final product physically rather than by chemical bond.[3] Due to this, OPEs leak into the environment more readily through volatilization, leaching, and abrasion. OPEs have been detected in diverse environmental compartments such as air, dust, water, sediment, soil and biota samples at higher frequency and concentration.[4]

II. Properties

(a) Bonding

The bonding in organophosphates has been a matter of prolonged debate; the phosphorus atom is classically hypervalent, as it possesses more bonds than the octet rule should allow.[5] The focus of debate is usually on the nature of the phosphoryl P=O bond, which displays (in spite of the common depiction) non-classical bonding, with a bond order somewhere between 1 and 2. Early papers explained the hyper-valence in terms of d-orbital hybridisation, with the energy penalty of promoting electrons into the higher energy orbitals being off-set by the stabilisation of additional bonding.[6]

(b) Acidity

Phosphate esters bearing P-OH groups are acidic. The pKa of the first OH group is typically Between 1-2, while the second OH deprotonates at a pKa between 6-7. As such, phosphate mono- and di-esters are negatively charged at physiological pH.[7] This is of great practical importance, as it makes these compounds far more resistant to degradation by hydrolysis or other forms of nucleophilic attack, due to electrostatic repulsion between negative charges. This effects nearly all organophosphate biomolecules, such as DNA and RNA and accounts in-part for their high stability. The presence of this negative charge also makes these compounds much more water soluble. [8]

(c) Water solubility

The water solubility of organophosphates is an important characteristic in biological, industrial and environmental settings. The wide variety of substitutes used in organophosphate esters results in great variations in physical properties. OPEs exhibit a wide range of octanol /water partition coefficients where log K values range from -0.98 up to 10.6. Mono- and di- esters are usually water soluble, particularity biomolecules. Tri-esters such as flame retardants and plasticisers have positive log K values ranging between 1.44 and 9.49, signifying hydrophobicity.[9] Hydrophobic OPEs are more likely to be bio accumulated and biomagnified in aquatic ecosystems. Halogenated organophosphates tend to be denser than water and sink, causing them to accumulate in sediments.[10]

(d) Industrial materials-

Organophosphates are best known for their use as pesticides. The vast majority are insecticides and are used either to protect crops, or as vector control agents to reduce the transmission of diseases spread by insects, such as mosquitoes. Health concerns have seen their use significantly decrease since the turn of the century.[11] Glyphosate is sometimes called an organophosphate, but is in-fact a phosphonate. Its chemistry, mechanism of toxicity and end-use as a herbicide are different from the organophosphate insecticides.[12]

(e) Flame retardants

Flame retardants are added to materials to prevent combustion and to delay the spread of fire after ignition. Organophosphate flame retardants are part of a wider family of phosphorus-based agents which include organic phosphonate and phosphinate esters, in addition to inorganic salts.[13-14] When some prominent brominated flame retardant were banned in the early 2000s phosphorus-based agents were promoted as safer replacements. This has led to a large increase in their use, with an estimated 1 million tonnes of organophosphate flame retardants produced in 2018.[40] Safety concerns have subsequently been raised about some of these reagents,[15]

(f) Plasticisers

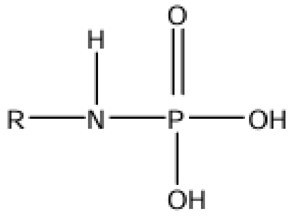
Plasticisers are added to polymers and plastics to improve their flexibility and process ability, giving a softer more easily deformable material. In this way brittle polymers can be made more durable. The most frequently plasticised polymers are the vinyl (PVC, PVB, PVA and PVCA), as well as cellulose plastics (cellulose acetate, nitrocellulose and cellulose acetate butyrate). PVC dominates the market, consuming 80-90% of global plasticiser production.[16] PVC can accept large amounts of plasticiser; it is common for products to be 0-50% plasticiser by mass, but loadings can be as high as 70-80% in the case of plastisol.[17]

Pure PVC is more than 60% chlorine by mass and is difficult to burn, but its flammability increases the more it is plasticised.[18] Organophosphates find use because they are multifunctional; primarily plasticising but also imparting flame resistance. Compounds are typically triaryl or alkyl diaryl phosphates, with cresyl diphenyl phosphate and 2-ethylhexyl diphenyl phosphate being important examples respectively.[19] These are both liquids with high boiling points. Organophosphates are more expensive than traditional plasticisers and so tend be used in combination with other plasticisers and flame retardants.[20]

III. Types of Organophosphate Esters (OPEs)

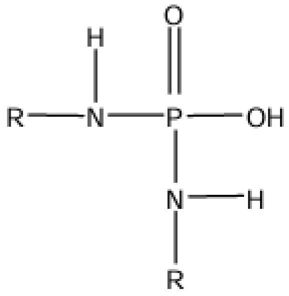
1. Mono-substituted phosphate ester (Mono-esters):

A mono-organophosphate ester is a phosphate ester where only one of the three hydroxyl groups (O-H) of phosphoric acid has been replaced by an organic group (R). These esters have the general formula O=P(OR), where "R" represents an alkyl or aryl group. They are a type of organophosphate, a broader class of compounds that include tri- and di-esters as well. [21]



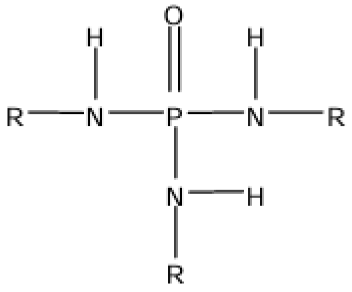
2. Di-substituted phosphate ester (di-esters):

Di-organophosphates, also known as di-organophosphate esters or di-OPEs, are a class of chemical compounds that are the esters of phosphoric acid with two organic groups attached to the phosphorus atom. They are related to tri-organophosphates (tri-OPEs) and some di-OPEs have been found to be more toxic than their corresponding tri-OPEs. Di-OPEs are commonly found in the environment and can be produced through the hydrolysis or degradation of tri-OPEs. [22]



3. Tri-substituted phosphate ester (tri-ester):

Tri organophosphate esters, also known as organophosphate tri-esters (tri-OPEs), are phosphate esters with three organic groups attached to the central phosphate molecule. They are widely used as flame retardants, plasticizers, and other additives in various products. Due to their widespread use and potential for environmental release, tri-OPEs have become a focus of environmental and health research. [23]



IV. Applications-

1. **Intermediates in Organic Synthesis:**

2,6-Dichloro-3-methylaniline serves as a building block in the synthesis of various organic compounds, including pharmaceuticals and agrochemicals.

2. **Pharmaceutical Intermediates:**

It is used in the development and synthesis of drug molecules, particularly in the creation of new drug candidates.

3. **Biochemical Research:**

It is used in proteomics research, according to Santa Cruz Biotechnology.

4. **ANDAs and Toxicity Studies:**

The compound is involved in the process of filing an Abbreviated New Drug Application (ANDA) with the FDA, which is a simplified process for generic drugs. It is also used in toxicity studies to evaluate the safety and potential adverse effects of new drug formulations.

5. R&D and Safety:

It is used in research and development (R&D) for pharmaceutical and chemical applications. It is also used in safety studies to assess the potential hazards of chemicals.

6. Other Applications:

It can be used as a reagent in various chemical processes and for the synthesis of dyes, as indicated by various sources.

In summary, 2,6-dichloro-3-methylaniline is an organic compound with a substituted benzene ring, commonly used as an intermediate in various chemical reactions, particularly in organic synthesis and pharmaceutical applications. [24]

V. Physicochemical Techniques for the Characterization of Complexes

The various analytical methods which were used for the characterization and structure elucidation of the synthesized Organophosphate Esters (OPEs) are given below.

- UV-Vis spectroscopy
- Infra-red spectroscopy (FTIR)
- Proton magnetic resonance spectroscopy (HNMR)
- Mass spectroscopy

A brief discussion of these methods is given below.

5.1 UV-Vis spectroscopy

UV-Vis spectroscopy is an analytical technique that measures the amount of discrete wavelengths of UV or visible light that are absorbed by or transmitted through a sample in comparison to a reference or blank sample. This property is influenced by the sample composition, potentially providing information on what is in the sample and at what concentration. Since this spectroscopy technique relies on the use of light, let’s first consider the properties of light.

Light has a certain amount of energy which is inversely proportional to its wavelength. Thus, shorter wavelengths of light carry more energy and longer wavelengths carry less energy. A specific amount of energy is needed to promote electrons in a substance to a higher energy state which can detect as absorption. Electrons in different bonding environments in a substance require a different specific amount of energy to promote the electrons to a higher energy state. This is why the absorption of light occurs for different wavelengths in different substances. Humans are able to see a spectrum of visible light, from approximately 380 nm, which we see as violet, to 780 nm, which we see as red.1 UV light has wavelengths shorter than that of visible light to approximately 100 nm. Therefore, light can be described by its wavelength, which can be useful in UV-Vis spectroscopy to analyse or identify different substances by locating the specific wavelengths corresponding to maximum absorbance (see the Applications of UV-Vis spectroscopy section). [25]

The Principle of UV-Visible Spectroscopy is the idea that chemical compounds can absorb ultraviolet or visible light, creating distinct spectra in the process. The basis of spectroscopy is the interaction of light and matter. A spectrum is created when the substance absorbs the light through excitation and de excitation processes.

The electrons existing in matter experience excitation when it absorbs UV energy. As a result, they move abruptly from their ground state (an energy condition with a negligible amount of energy) to their excited state (an energy state with a relatively large amount of energy associated with it). It is significant to remember that the amount of ultraviolet or visible radiation absorbed by an electron is always equal to the energy difference between its ground state and excited state.

The Beer-Lambert Law is the basic principle of absorbance spectroscopy. For a single wavelength, the following formulas are used: A = absorbance (unit less, commonly shown as arb. units or arbitrary units), a = molar absorptivity (M -1 cm-1) b = path length of the cuvette or sample container (usually 1 cm), and c= concentration of the solution (M). [26]

A = a b c

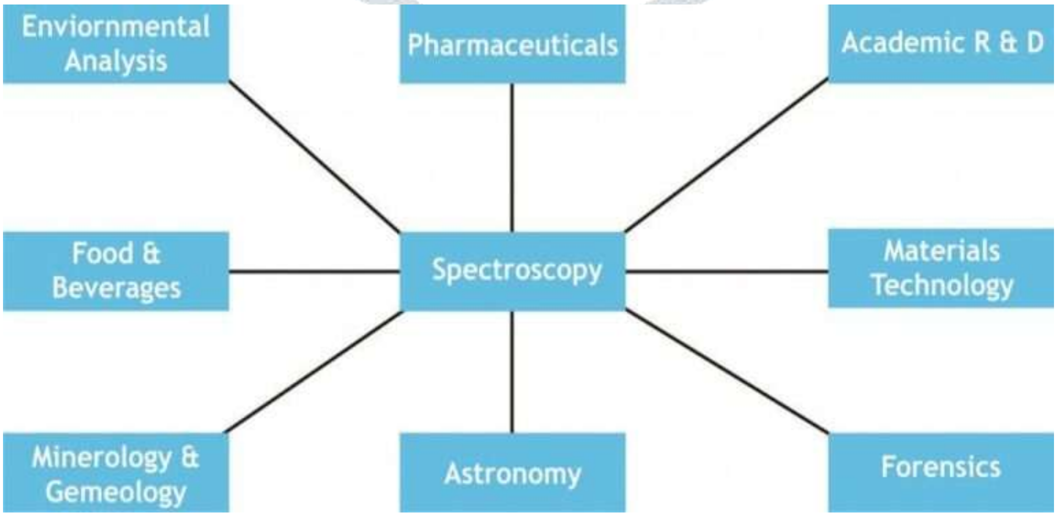
Where,

A: Absorbance a: Absorptivity b: path length c: Concentration

C: A /a b

Applications of UV-Vis spectroscopy -

UV-Vis spectrophotometry is widely used in many different scientific fields. Among the numerous noteworthy uses are protein and nucleic acid analysis, chemical analysis, and many more. Below are some of the widely used applications:



Applications of UV-Vis Spectrophotometer

- **Chemical Analysis**: Biomolecules, organic chemicals, and inorganic metals are commonly quantified in educational and industrial materials science labs using UV-Vis spectrophotometry. Its simplicity and speed of use make it a preferred method.

- **Nucleic acid and protein analysis**: UV-Vis spectrophotometry provides precise protein and nucleic acid concentration measurements, which is critical for applications in molecular biology, biochemistry, and genetics. For convenience of usage, many instruments include colors and protein types preconfigured or defined.
- **Pharmaceutical research**: UV-Vis spectrophotometry is an essential tool in the pharmaceutical business for identifying and quantifying chemicals in pharmaceutical products to ensure their efficacy and purity.
- **Purity Testing**: DNA samples are evaluated for purity using UV-Vis spectrophotometry, which guarantees that the samples are suitable for downstream processes like PCR and DNA sequencing.
- **Micro volume analysis**: Modern UV-Vis spectrophotometers are appropriate for small sample volumes because of technological improvements that allow them to analyse micro volume samples as little as 0.5 microliters.
- **Quality control analysis**: To ensure the quality and uniformity of ingredients and products, the approach is frequently employed in industries including food, cosmetics, and pharmaceuticals.
- **DNA and RNA analysis:** It focuses on verifying the concentration and purity of DNA and RNA, which plays a crucial role in downstream applications like sequencing. It ensures whether the DNA or RNA samples prepared for sequencing are contaminant or pure. Since pure DNA has an absorbance ratio of 1.8 and pure RNA has a ratio of 2, the 260 nm/280 nm absorbance ratio is crucial for displaying protein contamination in nucleic acids. 260nm/230nm absorbance ratio varies for RNA and DNA (2.15 to 2.50)**.**
- **Pharmaceutical analysis:** It is essential in drug discovery and development, quantifying impurities in drug ingredients, dissolution testing of solid oral dosage forms like tablets, and chemical identification and quantification. It allows overlapping absorbance peaks in the original spectra using mathematical derivatives to identify pharmaceutical compounds. Likewise, the Identification of pharmaceutical compounds, Chlortetracycline (antibiotic) and benzocaine in veterinary powder formulation, by overlapping the absorbance peaks in UV spectra using mathematical derivatives**.**
- **Food and Beverage Applications:** It applies to assessing the sensory attributes, nutritional components of food and its products such as beer, wine, juices, energy and soft drinks, waters, other thin liquids and thick liquids (honey, oils), fruits, vegetables, caffeine content, etc., and the chemical composition of ingredients and detect contaminants or adulterant to ensure the product is safe and healthier. It can be used in quality control in wine by identifying anthocyanin in blueberries, raspberries, and cherries. It can evaluate food and food product colour, flavour, and aroma**.**
- **Bacterial culture:** It is essential in the biomass growth curve. It is used in culturing bacteria by estimating cell concentrations and growth tracking in measuring optical density at 600 nm. 600 nm is best to preserve the optical properties of culture media where bacteria grow and to avoid cell damage when there is a need for continuous experimentation**.**

- **Other Applications**

1. In the cosmetic industry, it is used to evaluate photo stability agents and colour index, quantify dyes and antioxidants, and detect adulteration.

2. It is used in material science, like the characterization of small nanoparticles and to determine battery composition.

3. It is used to examine structural protein changes by tracking changes in peak wavelength absorbance.

4. In wastewater treatment, it is employed in kinetics and monitoring studies of dyes and dye by-products to ensure adequate dye removal by comparing their spectra over time.

5. It is used in cancer research to estimate haemoglobin concentration.

6. It is used to measure colour index to monitor transformer oil as a preventive measure to ensure electric power is delivered safely.

7. It is used in petro chemistry for characterizing crude oil, quality of crude oil gravity, formulation of indices for aromatic content, and sulphur content. [27]

5.2. Infra-red spectroscopy (IR)

The method known as infrared (IR) spectroscopy is based on a molecule's atoms vibrating. Typically, an IR spectrum is produced by exposing a material to IR radiation and measuring the percentage of incident radiation that is absorbed at a given energy. The frequency of a sample molecule's vibrational portion is correlated with the energy at which any peak in the absorption spectrum emerges.

A molecule needs to have a certain quality in order to exhibit IR absorptions: Throughout the movement, the molecule's electric dipole moment must change. Changes in molecular dipoles connected to vibrations and rotations can help explain how infrared radiation interacts with matter. Molecules contain atoms that can shift with respect to one another. This can happen when bond lengths change or when an atom moves off of its current plane. This is an explanation of the bending and stretching motions that are referred to as vibrations in general. Either a change in bond angle (bending) or bond length (stretching) can cause vibrations. Certain bonds have the ability to expand symmetrically (in phase) or asymmetrically (out of phase). The two stretching modes of a molecule with distinct terminal atoms will have different amounts of the stretching motion of each group rather than being symmetric and asymmetric vibrations of comparable bonds. Stated otherwise, the degree of connection will differ.

Even relatively basic molecules will have a wide variety of vibrations. Skeletal vibrations are vibrations that are coupled throughout a significant portion of the molecule or over its entirety, and this is what gives an IR spectrum its complexity. Instead of aligning with a particular group inside the molecule, bands linked to skeletal vibrations are more likely to follow the pattern or fingerprint of the molecule as a whole.

The electromagnetic spectrum of IR is commonly classified into three regions: near 14000-4000 cm^{-1} (0.8-2.5 um), mid 4000-400 cm^{-1} (2.5-25 um), and far infrared 400 cm^{-1} (25-1000 um). An extremely elegant and powerful tool for the elucidation of molecular structure has been provided to physicists and chemists by the feature of characteristic absorption of radiations by many molecules in IR region. In the infrared portion of the spectrum, absorption bands are created by the excitation of molecule rotation and vibration. The arrangement of atoms in space, their masses, bond lengths, bond angles, and the force between the two atoms all affect the spectrum.

The atomic groups in a molecule undergo twisting, bending, rotating, and vibrational motions during infrared spectroscopy. Only non-centrally symmetric vibrations are infra-red active. A molecule's infrared spectrum is the result of transitions between two distinct vibrational energy levels. The vibrational energy of a chemical bond is quantized and can have the value.

$$E_{vib} = [\upsilon + 1/2]h\upsilon$$

Where, υ is the number of the vibrational level and can have the values 0,1,2,3........

h = Planck’s constant

v = Vibrational frequency of a bond

For harmonic oscillation, frequency is related to the force constant and the reduces mass by the Hooke’s law relationship:

$$V/c = \tilde{\upsilon} = 1/2\pi c\ [k/m_1m_2/m_1m_2]^{1/2} = 1/2\ \pi c\ \sqrt{k/\mu}$$

Where, μ is the reduced mass, m and m are the masses of the atoms concerned in grams in a particular bond

k = Force constant in dynes/cm

c = Velocity of radiation

$\tilde{\upsilon}$ = Wave number of an absorption peak in cm^{-1}

Thus, the vibrational frequency (or wave number) depends upon strength and reduced mass. [110]

Applications of Infra-red spectroscopy -

- Structure Elucidation and Functional Group Identification:

IR spectroscopy allows for the identification of specific functional groups within molecules, providing insights into their structure.

- Compound Identification:

IR spectra are unique to each compound, enabling the identification of unknown substances.

- Reaction Monitoring:

By observing changes in absorption bands, IR spectroscopy can track the progress of chemical reactions.

- Quality Control and Purity Testing:

IR spectroscopy can be used to verify the purity of raw materials, finished products, and incoming goods.

- Pharmaceutical Applications:

It's used to analyse drug identity, test purity, and study interactions between active ingredients and excipients.

- Environmental Monitoring:

IR spectroscopy is employed to detect pollutants in air and water, as well as monitor air quality.

- Materials Science:

IR spectroscopy is used to analyse the composition and structure of materials, including polymers and semiconductors.

- Food Industry:

It's used to measure the concentration of various compounds in food products.

- Protein Characterization:

IR spectroscopy is used to study the structure and conformation of proteins.

- Space Exploration:

IR spectroscopy is used in space exploration to analyze planetary atmospheres and other extra-terrestrial samples. [28]

5.3 Nuclear Magnetic Resonance Spectra

NMR is a quantitative spectroscopic method since the intensity of the peaks is proportional to the number of nuclei. NMR sensitivity and resolving power have improved as electronics have developed and stronger magnetic field strengths have been used. However, the lack of established protocols has limited its quantitative application, and many people see NMR as primarily a qualitative technology, used for chemical structure determination and molecular dynamics**.** In principle, the substance might be placed in a magnetic field of constant strength, and the spectrum could then be acquired by transmitting radiation with a constantly changing frequency through the substance and monitoring the frequency at which radiation is observed. In reality, however, it has been discovered to be more convenient to maintain the radiation frequency while varying the strength of the magnetic field. At some degree of field strength, the energy required to flip the proton equals the energy of the radiation, resulting in absorption and a signal. Such a spectrum is known as a nuclear magnetic resonance (NMR) spectrum.

It is commonly known that all nuclei are positively charged. In some nuclei, this charge spins on the nuclear axis, causing a magnetic dipole to form along the axis. As a result, the nucleus functions similarly to a small bar magnet. The spinning charge's angular momentum is defined by its nuclear magnetic moment (μ). The spinning nucleus of a hydrogen atom (1H or proton) is the simplest and most usually found in organic molecules. The hydrogen nucleus has a magnetic moment (μ=1/2). As a result, in the presence of an external magnetic field, Ho's magnetic moment can have two orientations. The orientations in which the magnetic moment is parallel to the applied magnetic field are more stable (lower energy). The difference in energy (ΔE) between the two states determines the energy needed to flip the proton from its lower energy alignment to the higher energy alignment. This energy is equal to hυ ($\Delta E = h\upsilon$). Given an electromagnetic frequency and a magnetic field strength, the basic NMR equation is

$$\upsilon = \gamma H_o/2\pi \text{............ (A)}$$

Where, υ = frequency in cycles/second

H_o = strength of applied field in gauss

Γ = gyromagnetic ratio or nuclear constant.

The precessional angular velocity, $\dot{\omega}_o$ is equal to the product of the gyromagnetic ratio, γ and strength of the applied field, H_o

$$\dot{\omega}_o = \gamma H_o \ldots\ldots\ldots\ldots\ldots \text{(B)}$$

From equation A and B

$$\gamma H_o = 2\pi\upsilon$$

Therefore,

$$\dot{\omega}_o = 2\pi\upsilon$$

The most crucial method for characterizing organic compounds is proton magnetic resonance (PMR) spectroscopy, which provides information on the many contexts in which the hydrogen atoms in a molecule are found. In addition, PMR provides information on the nature of protons (based on the signal's position in the spectrum) and the quantity of protons of each type (based on the number of peaks in the spectrum). [29]

Applications of NMR spectroscopy -

➢ Chemical Structure Determination:

NMR is a powerful tool for identifying the structure of organic and inorganic compounds. By analyzing the chemical shifts, splitting patterns, and integration values in an NMR spectrum researchers can gain insights into the connectivity of atoms and functional groups within a molecule.

➢ Molecular Dynamics and Interactions:

NMR can be used to study the motion and dynamics of molecules, including the orientation and motion of individual atoms and groups of atoms. It can also be used to investigate intermolecular interactions, such as hydrogen bonding and van der Waals forces.

➢ Biological Systems:

NMR is widely used in biochemistry and structural biology to study the structure and function of biological macromolecules, including proteins, nucleic acids, and carbohydrates. It can also be used to study metabolic pathways and biomarker discovery.

➢ Metabolomics:

NMR spectroscopy is used to analyze the composition of metabolites in biological samples. This can provide valuable information about metabolic pathways and can be used to identify biomarkers for disease diagnosis.

➢ Materials Science:

NMR is applied in materials science to investigate the structure and properties of materials, including polymers, catalysts, and nanomaterials.

➢ Food Science:

NMR is used in food science to determine the structure and composition of food components, such as proteins, lipids, carbohydrates, and amino acids. It can also be used to assess the quality and safety of food products.

➢ Medicine and Diagnostics:

NMR plays a crucial role in medical imaging, such as Magnetic Resonance Imaging (MRI), which is based on the same principles as NMR spectroscopy. It can also be used for noninvasive analysis of living organisms and in the diagnosis of various diseases.

➢ Pharmaceutical Analysis:

NMR is used in pharmaceutical research for drug development, quality control, and analysis of excipients. It can help determine the purity, content, and molecular structure of pharmaceutical compounds.

➢ Environmental Science:

NMR is used in environmental science to study the composition and properties of humic substances in soil and water. It can also be used to monitor environmental pollution and assess the degradation of pollutants.

➢ Forensic Science:

NMR can be used in forensic science to identify and analyze unknown substances found at crime scenes, such as drugs and poisons. [30]

5.4 Mass Spectrometry

Utilizing mass spectrometry, one may ascertain a compound's elemental composition and molecular mass analytically. Spectra are utilized in the identification of elemental or isotopic composition of a sample, as well as in the determination of particle and molecular masses and the clarification of chemical structures of substances such as peptides.

Basically through electron ionization, the process of producing gas phase ions of a substance is the initial step in the mass spectrometric study of molecules. There is fragmentation of this molecular ion. Fragmentation occurs in each primary product ion that is produced from the molecular ion, and so on. Using this method, molecules are subjected to an intense electron beam that transforms them into highly charged ions known as molecular ions or parent ions. These ions have the ability to fragment or form daughter ions, which are smaller ions.

In the mass spectrometer, the ions are detected in proportion to their abundance after being separated based on their mass-to-charge ratio. Ions will deflect to the same degree if their mass to charge ratio is the same. This results in the creation of the molecule's mass spectrum. The outcome is shown as a plot of ion abundance against mass-to-charge ratio. Ions reveal details about the composition and structure of the molecule that came before them.

If present, the molecular ion yields the molecular mass of the compound and appears at the highest value of m/z in the spectrum of a pure compound, followed by ions with heavier isotopes.

The mass spectrometer consists of three major components:

1) Ion Source: For producing gaseous ions from the substance being studied.

2) Analyser

: For resolving the ions into their characteristics mass components according to their mass-to-charge ratio.

3) Detector System: For detecting the ions and recording the relative abundance of each of the resolved ionic species**.**

During electron bombardment, the sample molecules can react in two different ways: either they absorb an electron and produce a radical anion, or they remove an electron and produce a radical cation .

M --------------------- M^{-} electron capture

M----------------------M^{+} + 2^{e-}

Deciding what kinds of samples mass spectrometry can analyse has mostly depended on ionization techniques. Gases and vapours are ionized chemically or via electronization. Chemical ion-molecule reactions occur in chemical ionization sources, ionizing the analyte during source collision. Efficient electrons interact with gas phase atoms or molecules to form ions through the process of electron ionization. Especially for gasses and volatile organic compounds, mass spectrometry uses this technique extensively.

In an EI ion source, electrons are produced through thermo ionic emission by heating the filament that has electric current running through it. The electrons are accelerated to 70 eV in the region between the filament and the entrance to the ion source block. The accelerated electrons are then concentrated into the beam by being attracted to the trap electrode. The samle under investigation which contains the neutral molecules is introduced to the source in a perpendicular direction to the electron beam. Close passage of highly energetic electrons, referred to as a hard ionization source, causes the large fluctuations in the electric field around the neutral molecules and induces the ionization and fragmentation**.** [31]

Applications of Mass spectroscopy –

➢ Mass spectrometry in proteomics –

Characterization of proteins and protein complexes, sequencing of peptides, and identification of posttranslational modifications.

➢ Mass spectrometry in metabolomics –

Cancer is screening and diagnosis, global metabolic fingerprinting analysis, biomarker discovery and profiling, biofuels generation and use, lipidomics studies, and metabolic disorder profiling.

➢ Mass spectrometry in environmental analysis –

Drinking water testing, pesticide screening and quantitation, soil contamination assessment, carbon dioxide and pollution monitoring, and trace elemental analysis of heavy metals leaching.

➢ Mass spectrometry in pharmaceutical analysis –

Drug discovery and absorption, distribution, metabolism, and elimination (ADME) studies, pharmacokinetic and pharmacodynamic analyses, metabolite screening, and preclinical development.

➢ Mass spectrometry in forensic analysis –

Analysis of trace evidence (e.g., fibers in carpet, polymers in paint), arson investigation (e.g., fire accelerant), confirmation of drug abuse, and identification of explosive residues (bombing investigation).

➢ Clinical applications of mass spectrometry –

Clinical drug development, Phase 0 studies, clinical tests, disease screening, drug therapy monitoring, analysis of peptides used for diagnostic testing, and identification of infectious agents for targeted therapies. [32]

VI. **CUNCLUSION**

Organophosphrus compounds have tremendous importance in the field of food technology, animal foodstuffs, pesticides, Medicinal compounds, synthetic polymers, fire retardants and natural product. All the synthesize compounds were characterized by using analytical data obtained from IR, 'HNMR, UV Spectroscopy and Mass Spectroscopy.

REFERENCES

1. Greaves, A. K., Letcher, R. J., Chen, D., McGoldrick, D. J., Gauthier, L. T., & Backus, S. M. (2016). Retrospective analysis of organophosphate flame retardants in herring gull eggs and relation to the aquatic food web in the Laurentian Great Lakes of North America. Environmental Research, 150, 255-263.
2. Ung, S. P. M., & Li, C. J. (2023). From rocks to bioactive compounds: a journey through the global P (V) organophosphorus industry and its sustainability. RSC Sustainability, 1(1), 11-37.
3. Wang, X., Zhong, W., Xiao, B., Liu, Q., Yang, L., Covaci, A., & Zhu, L. (2019). Bioavailability and biomagnification of organophosphate esters in the food web of Taihu Lake, China: Impacts of chemical properties and metabolism. Environment International, 125, 25-32.
4. Wei, G. L., Li, D. Q., Zhuo, M. N., Liao, Y. S., Xie, Z. Y., Guo, T. L., ... & Liang, Z. Q. (2015). Organophosphorus flame retardants and plasticizers: sources, occurrence, toxicity and human exposure.

Environmental pollution, 196, 29-46.

5. Fugel, M., Malaspina, L. A., Pal, R., Thomas, S. P., Shi, M. W., Spackman, M. A., ... & Grabowsky, S. (2019). Revisiting a historical concept by using quantum crystallography: Are phosphate, sulfate and perchlorate anions hypervalent? Chemistry–A European Journal, 25(26), 6523-6532.
6. Cundari, T. R. (2013). Chemical bonding involving d-orbitals. Chemical Communications, 49(83), 9521-9525.
7. BD, D. (1958). On the importance of being ionized. Archives of Biochemistry and Biophysics, 78(2), 497-509.
8. Westheimer, F. H. (1987). Why nature chose phosphates. Science, 235(4793), 1173-1178.
9. Greaves, A. K., & Letcher, R. J. (2017). A review of organophosphate esters in the environment from biological effects to distribution and fate. *Bulletin of environmental contamination and toxicology*, *98*, 2-7.
10. McDonough, C. A., De Silva, A. O., Sun, C., Cabrerizo, A., Adelman, D., Soltwedel, T., ... & Lohmann, R. (2018). Dissolved organophosphate esters and polybrominated diphenyl ethers in remote marine environments: Arctic surface water distributions and net transport through Fram Strait. *Environmental science & technology*, *52*(11), 6208-6216.
11. World Health Organization, UNEP United Nations Environment Programme, & World Organisation for Animal Health. (2022). One health joint plan of action (2022–2026): working together for the health of humans, animals, plants and the environment. World Health Organization.
12. van den Berg, H., da Silva Bezerra, H. S., Al-Eryani, S., Chanda, E., Nagpal, B. N., Knox, T. B., ... & Yadav, R. S. (2021). Recent trends in global insecticide use for disease vector control and potential implications for resistance management. Scientific reports, 11(1), 23867.
13. Van der Veen, I., & de Boer, J. (2012). Phosphorus flame retardants: properties, production, environmental occurrence, toxicity and analysis. Chemosphere, 88(10), 1119-1153.
14. Schmitt, E. (2007). Phosphorus-based flame retardants for thermoplastics. Plastics, Additives and Compounding, 9(3), 26-30.
15. He, H., Gao, Z., Zhu, D., Guo, J., Yang, S., Li, S., ... & Sun, C. (2017). Assessing bioaccessibility and bioavailability of chlorinated organophosphorus flame retardants in sediments. Chemosphere, 189, 239-246.
16. Blum, A., Behl, M., Birnbaum, L. S., Diamond, M. L., Phillips, A., Singla, V., & Venier, M. (2019). Organophosphate ester flame retardants: are they a regrettable substitution for polybrominated diphenyl ethers?. Environmental science & technology letters, 6(11), 638-649.
17. Rahman, M., & Brazel, C. S. (2004). The plasticizer market: an assessment of traditional plasticizers and research trends to meet new challenges. Progress in polymer science, 29(12), 1223-1248.
18. William Coaker, A. (2003). Fire and flame retardants for PVC. Journal of Vinyl and Additive Technology, 9(3), 108-115.
19. Grossman, R. F. (Ed.). (2008). Handbook of vinyl formulating. John Wiley & Sons.
20. Levchik, S. V., & Weil, E. D. (2005). Overview of the recent literature on flame retardancy and smoke suppression in PVC. Polymers for advanced technologies, 16(10), 707-716.
21. Wéry, J., Radelicki, S., Hooper, T. J., Houbrechts, M., Janssens, K., Stuyck, W., ... & De Vos, D. E.

(2025). Selective synthesis of phosphate mono-esters with an acidic modified niobium oxide catalyst. Tetrahedron Green Chem, 5, 100063.

22. Bunton, C. A., & Ionescu, L. G. (1973). Hydrolysis of di-and trisubstituted phosphate esters catalyzed by nucleophilic surfactants. *Journal of the American Chemical Society*, *95*(9), 2912-2917.

23. Pozzi, G., Colombani, I., Miglioli, M., Montanari, F., & Quici, S. (1997). Epoxidation of Alkenes Under Liquid-Liquid Biphasic Conditions: Synthesis and Catalytic Activity of Mn (III)-Tetraarylporphyrins Bearing Perfluoroalkyl Tails. Tetrahedron, 53(17), 6145-6162.