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Tawseef Ahmad Bhat
Department of Chemistry, Madhyanchal Professional University (MPU) - Educational Institute, Bhopal, Madhya Pradesh, India

Vinay Kumar Jain
Department of Chemistry, Madhyanchal Professional University (MPU) - Educational Institute, Bhopal, Madhya Pradesh, India

Zahoor Ahmad Malik
School of Pharmaceutical Sciences, RGPV, Bhopal, Madhya Pradesh India

Corresponding Author:
Tawseef Ahmad Bhat
Department of Chemistry, Madhyanchal Professional University (MPU) - Educational Institute, Bhopal, Madhya Pradesh, India

Synthesis of Tri-(4-Chlorothio) phenyl phosphate ester and its characterization from IR absorption spectra

Tawseef Ahmad Bhat, Vinay Kumar Jain and Zahoor Ahmad Malik

Abstract
Tri-4-chlorothiophenyl phosphate ester has been synthesized by Auger and Dupis method in a ratio of 1:1 thiol and POCl3. The compound has been characterized by IR absorption spectra and elemental detection. The spectral study was conducted on KBr disc. IR spectra of Di-4-chlorothiophenyl phosphate ester clearly reveals different stretching frequencies of almost all the bonds present in the compound at their respective wave numbers. The study of orthophosphate esters has been intensively taken into consideration in recent years due to their significant role in various realms of human interest. Thiophosphate esters have been used as lubricant additives for over 50 years. They also find their use as surfactants and brighteners in detergents. They have an important role in chemistry and in biochemistry as they possess common linkages to those present in nucleotides.

Keywords: Tri-4-chlorothiophenyl phosphate, Auger and Dupis, absorption spectra, elemental detection, stretching

Introduction
The ester of phosphoric acid is referred to as an organophosphate. The most common organophosphorus chemical is probably phosphate. Due to their numerous uses in the analytical (Quin, 2000, and Audrieth & Toy, 1942) [1, 2], biological (Holmstedt, 1959 and Arnold *et al*., 1961) [3, 4], and industrial (Moss and Morales, 2001) [5] sectors, phosphate esters' chemistry continues to catch the interest of chemists. They are basically the building blocks of DNA and protoplasm and are necessary to the survival of life. The value of phosphotes with C-S-P linkage cannot be overstated. They are utilised for biological research, insecticidal action (Gardner and Kilby, 1950) [7], radioactive tracer methods, antiviral activity (Schlesinger, 1955) [8], and textile products (Dayer, 1959) [9]. It is crucial to learn about their stability and bond cleavage due to their varied usage.

Material and Methods
The methods of synthesis of phosphate Tri-esters which are undertaken for kinetic study have been illustrated as follows:

Method of preparation
TRI-4-chlorothiophenyl phosphate
Tri-4-chlorothiophenyl phosphate has been prepared by using phosphorus penta chloride as phosphorylating Moss &Morales, 2001, Tonaka *et al*., 1974) [5, 6] agent. The ratio of 3: 1 of phenol and PCI_5 was employed for this preparation. 4.899 g of 4-chlorothiophenol (A.R. grade Sigma-Aldrich) was dissolved in 15 ml of dry benzene stirred well for few minutes. 1.30 ml of PCI_5 was added. Initially the reaction was very rapid and PCI_5 dissolved immediately and white insoluble material began to separate. Keeping it overnight and then dissolved it in a solvent and thus it was subjected to a steam distillation when aqueous and benzene layer were distilled off separately. The residue left after distillation was treated first with water and then with 10% NaOH solution to remove unreacted phenol (Table 1). A white residue insoluble in NaOH was obtained. It was washed with distilled water to remove Excess of alkali and crystallized from absolute alcohol. Shining crystals of Tri-4-chlorothiophenyl phosphate were obtained.

Table 1: Estimation of Elements

S. No	Element	Percentage	
		Theoretical	Observed
1.	Carbon	45.246	45.11
2.	Hydrogen	2.5314	2.325
3.	Chlorine	22.2589	21.908
4.	Phosphorus	6.4835	6.246
5.	Oxygen	3.3485	3.186
6.	Sulphur	20.1312	20.03

Results and Discussion

A thorough kinetic study of the hydrolysis of Tri-4-chlorothiophenyl phosphate has been carried out in acid {0.1 to 7.0 mol dm^{-3} HCl} and in buffer 1.24 to 7.46 pH at 98°. The kinetic study was performed in 10% aqueous dioxan (V/V). The solvent water-dioxan was used for the stability reason of the diester, since this is insoluble in water. The study has yielded pseudo-first order rate coefficients and the rate data is supported and interpreted by different kinetic evidences. Hydrolysis of the diester involves two stages to give inorganic phosphate. Di-4-chlorothiophenyl phosphate converted into their monoester which further undergo hydrolysis to form orthophosphoric acid. The diester has been found to show reactions via mononegative species, neutral species and conjugate acid species. The result shows that rate constant increases with decrease in polarity of the solvent. The reaction between two neutral molecules should involve a change in transition state and such a reaction should be easier in a more polar mixture. The abnormal reactivity of the neutral ester may not be presumed to undergo such a simple reaction between neutral ester and water molecule. The study of kinetics of phosphate esters can have different types of linkages such as C-S-P, C-N-P and C-O-P etc. which cover a vast range of human race development.

IR. Spectra

The compound was also identified from its characteristic absorption spectra in KBr disc. IR spectral data of Tri-4-chlorothiophenyl phosphate has been shown in Table 2 and Figure 1 (The spectral study was conducted on BRUKER Alpha FT- IR Spectrophotometer, SIRT Bhopal).

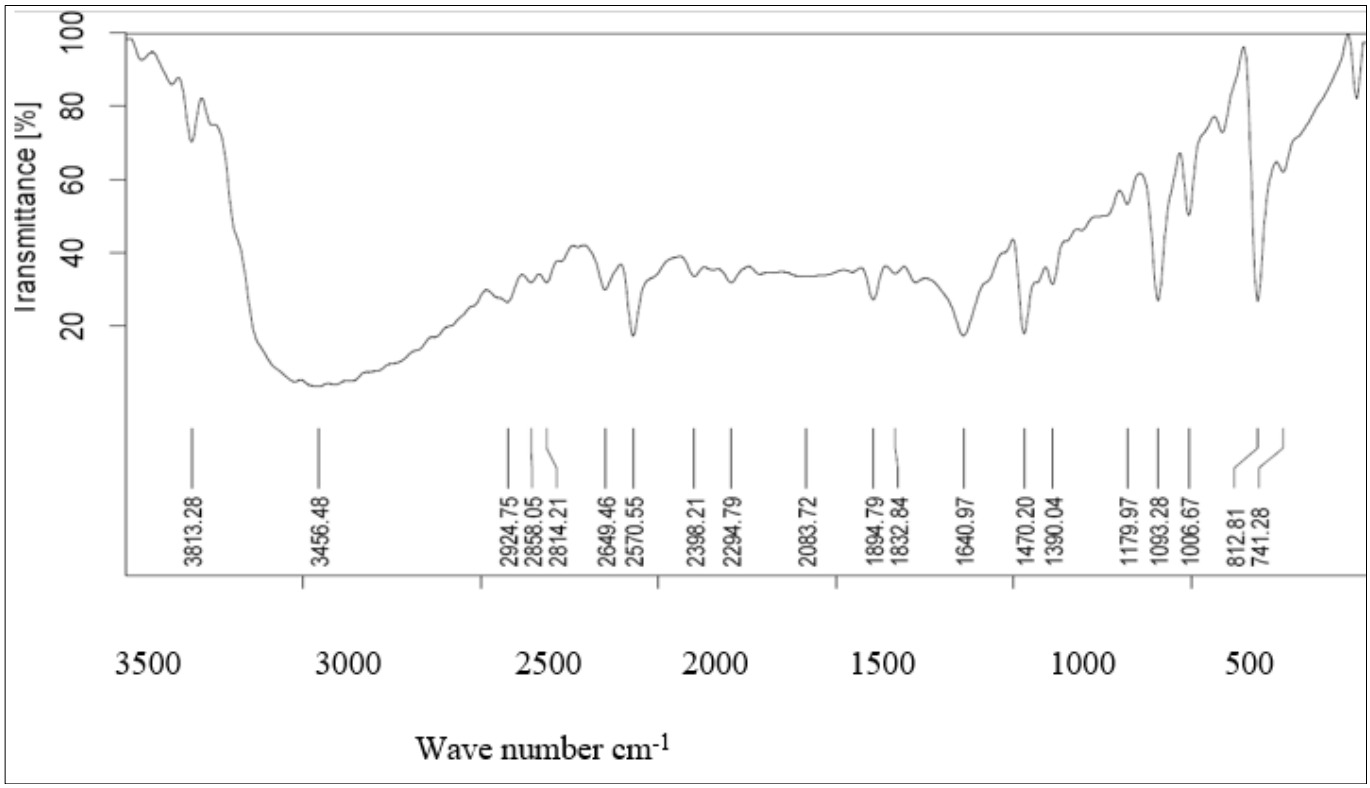

Fig 1: Shows IR Spectra of Triester chlorothiophenyl Phosphate

Table 2: IR Spectral Data of Triester-4-chlorothiophenyl Phosphate

S. No	V cm P-O Stretching	V cm^{-1} (O-H) stretching	IRv cm (P-S) stretching	IRv cm Ar(C=C) stretching	IRv cm (C-S) stretching	IRv cm Ar (C-CI) stretching
1.	812.81	3456.4792		1470.20	2570.55	1093.28

Conclusion

The study of orthophosphate esters has been intensively taken into consideration in recent years due to their significant role in various realms of human interest. Thiophosphate esters have been used as lubricant additives for over 50 years. They also find their use as surfactants and brighteners in detergents. They have an important role in chemistry and in biochemistry as they possess common linkages to those present in nucleotides. Determining their mechanism of hydrolysis reaction can give an important clue to trace out the path of complicated reactions including both chemical and enzymatic hydrolysis of phosphate esters which are of biological importance. Kinetic study on the hydrolysis of these esters can provide new reaction paths to the academicians too. Besides this, organic phosphates find their use as pesticides. These esters are also industrially and medicinally important.

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