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Synthesis of Di-(4-Chlorothio) Phenyl Phosphate Ester and its characterization from IR absorption spectra

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Abstract
Di-4-chlorothiophenyl phosphate ester has been synthesized by Auger and Dupis method in a ratio of 1:1 thiol and $POCl_3$. 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: Di-4-chlorothiophenyl phosphate, Auger and Dupis, absorption spectra, elemental detection, stretching

Introduction
An organophosphate refers to the ester of phosphoric acid. Phosphates are most probably the most prevalent organophosphorus compounds. The chemistry of phosphate esters continues to draw the attention of chemists due to their versatile applications in the analytical (Mhala *et al.*, 1977 and Bunnett, 1961) [1, 4], biological (Zucker & Hammett, 1939 and Bunnett, 1961) [3, 4] and industrial fields (Long & Paul, 1957 and Mhala *et al.*, 1970) [5, 6]. They are essentially the constituent components of DNA and protoplasm and play a vital role for the maintenance of life. Phosphates having C-S-P linkage are of great importance. They are used for antiviral activity (Bokil, 1970) [7], radioactive tracer techniques (Kadmane, 1971) [8], for biological investigations, insecticidal activity (Mhala and Prabha, 1972) [9] and textile commodities (Mhala & Jagdale, 1968) [10]. Due these multiple uses it is important to get knowledge about their stability and bond cleavage.

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

Method of preparation
Di-4-chlorothiophenyl phosphate
It was also prepared by Auger and Dupis method. 4-chlorothiophenol (A.R. grade) and $POCI_3$ were taken in 2:1 ratio. 7 ml of pyridine was added slowly to a stirred solution of 4-chlorothiophenol (6.52 g) and $P0CI_3$ (1.83 ml) in dry benzene (25 ml). Pyridine Hydrochloride began to separate immediately with the evolution of heat. The mixture was stirred on a magnetic stirrer at 60 to 65^0 for a period of 10 hrs. and 30 minutes. The yellowish oily residue left after stirring was treated with H_20 and then with 5% NaOH. The filtrate thus obtained was acidified with dilutes HCL to precipitate the chloride which on washing with distilled water was converted into the free diester. This free diester was finally dissolved in CCl_4 and filtered off to remove impurities

Results and Discussion
A thorough kinetic study of the hydrolysis of Di-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.

Table 1: Estimation of Elements

S. No	Element	Percentage	
		Theoretical	Observed
1.	Carbon	41.0377	40.94
2.	Hydrogen	2.5830	2.189
3.	Phosphorus	8.8207	8.790
4	Chlorine	20.1886	20.00
5	Oxygen	9.1111	8.923
6	Sulphur	18.2587	18.107

IR Absorption Spectra: The compound was also identified from its characteristic absorption spectra in KBr pellets. IR spectral data of Di 4-chloro thiophenyl phosphate has been shown in (Table 2 and Figure 1), (The spectral study was conducted on Bruker Alpha Ft-Ir Spectrophotometer).

Table 2: IR Spectral Data of Di-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.	815.01	3434.3701		14.68.30	2359.1401	1090.54

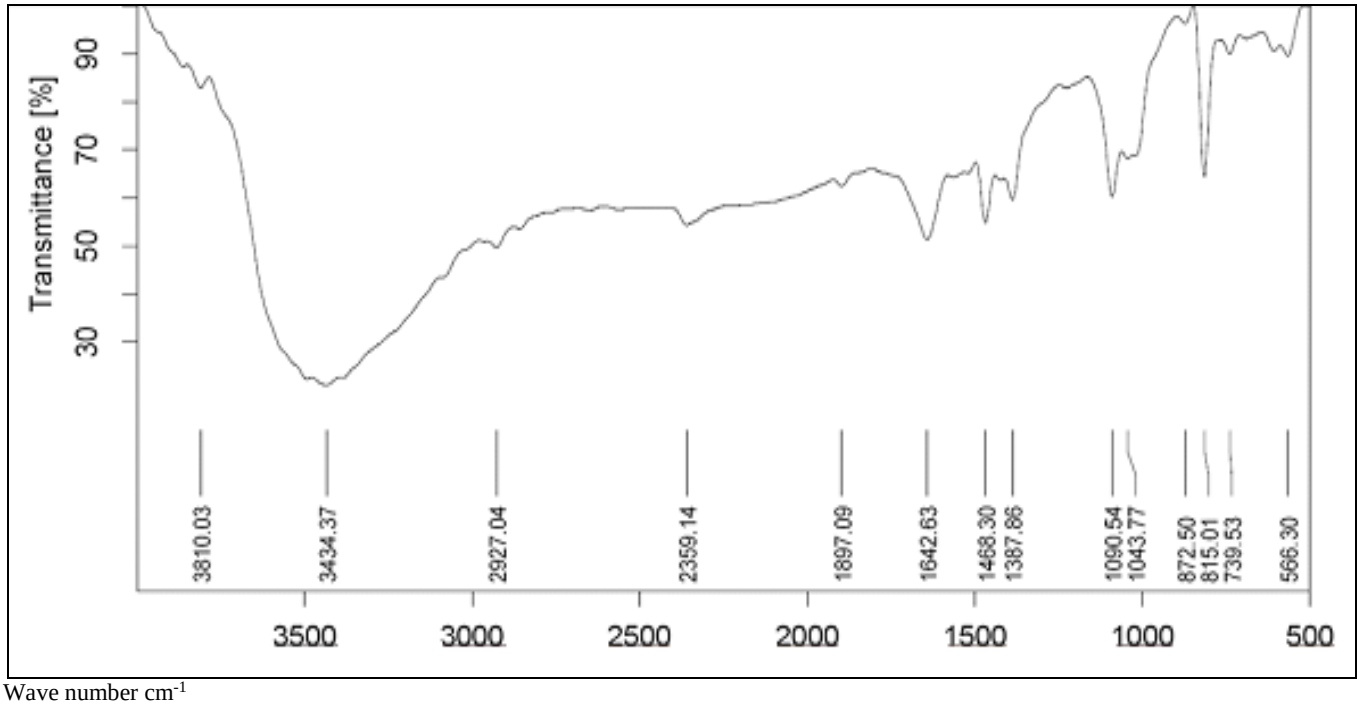

Fig 1: Shows IR Spectra of Diester chlorothiophenyl Phosphate

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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