

CATALYTIC HYDROLYSIS OF ORGANOPHOSPHATES BY MICELLAR ORGANO IODINANE OXI ANIONS

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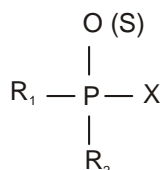
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Abstract—Organophosphate and phosphonate compound are used widely as pesticides in agriculture as chemical warfare agents and as flame retardants hydraulic fluids and plasticizers in industry. However some of these compounds are among the most noxious chemical known to mankind & destruction of phosphorus based nerve agents under battlefield. ("decontamination") 1, 2 or treaty mandata stock pile a matter of urgent concern. It is proposed to study the toxic organophosphates & phosphonates as Inhibitors of acetylcholine esterase.

Keywords: organophosphates, micellar organosulfonate oxianions.

INTRODUCTION

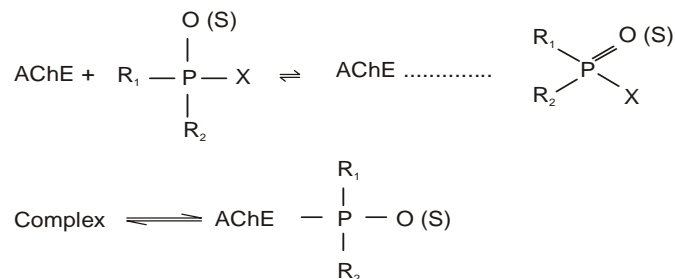
The General formula of an organophosphorus toxin is



Where R₁ & R₂ are groups which can not be easily displaced from phosphorus eg. Alkoxy alkyl or dialkyl amine amino) and X can function as a leaving group for example –

F or p-nitro phenoxy³

The ability of these comp. to inhibit the function of enzyme such as acetyl cholin esterase (AChE) form the basis of their activity as pesticides and chemical warfare agent. organophosphorus toxins and good phosphorylating agents. They normally function by esterifying the active site serine hydroxyl group of acetyl cholinesterase. Thus it is not surprising that attempts to develop useful decontaminants have concentrated on hydrolytic reagents for phosphates and phosphonates.



EXPERIMENTAL PROCEDURE

General method : M.P. are uncorrected

NMR—NMR were determined on a varian 200 MHz instrument,

PH. meter— Fisher module 320 digital ph meter (calomel electrode was used to adjust the ph of the solution).

MATERIALS USED

PNPDPP was prepared using a literature method⁴

CTATCI was obtained from aldrich. commercially available chemicals were used as received. For kinetics all buffers were prepared from steam distilled water preparation of 1, 3, dihydro 1-oxido-3-methyl-1, 2, 3, benziodoxy phospho-3-oxide-2-bromo aniline 24 (Reagent-22) was refluxed with acetic anhydride glacial acetic acid and Zn dust to get 2-bromo (acetanilide phosphinates⁵ was then prepared in 96% yield via anhydrous NaCl₂ catalyzed Arbuzov reaction⁶ of diethyl methyl phosphinate and 2-bromoacetanilide then the amino group of phosphinate was hydrolyzed, diazotized and converted to the aryl iodide.

RESULT AND DISCUSSION

1. **Pka determination** : The catalysis of phosphate cleavage is a property of the closed form of these idoso reagents so that the kinetic enhancement of PNPAPP cleavage must be attributed to the benziodoxathiole form.

the kinetic data are summarized in table –1

PH	10 ³ k _{cat} S ⁻¹ (22)	Log k _{cat} (22)
6.33	1.64	-2.786
6.6	2.16	-2.666
6.9	2.84	-2.546
7.15	2.87	-2.543
7.42	2.95	-2.529
8.07	3.25	-2.488
8.33	3.34	-2.476

2. **Kinetic study**—The catalytic properties of 22 were assessed from full rate constant (Surfactant) profiles for

the cleavage of 1×10^{-5} M, p-nitro phenyl diphenyl phosphate (PNPDPP) by 1×10^{-4} M catalyst at different CTACI conc. at $25 \pm 0.5^\circ\text{C}$ and given in table 2

Table 2: Rate constant for the cleavage of DNPDP as a function of CTACI conc.

10^2 (CTACI)M	10^3 k_{obs}^{-1} for 22
3.5	1.21
2.0	1.42
1.5	1.50
1.0	1.64
0.5	1.55
0.3	-
0.2	1.42
0.1	1.35
0.075	-
0.05	1.00
0.02	-
0.01	0.43

CONCLUSION

X Ray crystallographic data for reagent-22-OH reveals that they are about as closed as 14-OH. The endocyclic I-O Bonds were found to be 2.29 \AA^7 & 2.37 \AA^8 . The computed structural parameter describing the environment around the I atom are very sensitive to the computational level employed.

REFERENCES

- [1] Ember, L. R. Chem. Eng. News 1995 (Maron 27), 26 ibid 1994 (Aug 1; 1) ibid. 1994 (Feb. 14), 7.
- [2] Yang, Y.Ci; Baker, J.A.; Ward., J.R. Chem. Rev. 1992, 92, 1729
- [3] Emsley, J; Hall, D. "The Chemistry of phosphorous". Wiley; New York, 1976; pg494-509.
- [4] Moss, R.A.; chatterjee, 5; wilk, W.J. Org. Chem. 1986, 51, 4303.
- [5] Balthazor, T.M. Miles, J.A., Stults, B.R., J. Org. Chem. 1978, 93, 4538
- [6] March, J. Advanced Organic chem. Reactions, mechanisms and Structures, 4th edition 1992, Willey, New York, P-959
- [7] Balth azro, T.M.; Miles, J.A.; Stults, B.R., Org. Chem, 1978, 43, 4538
- [8] Koser, G.F.; Sun, G., Porter, C.W., Youngs, W.J. J. Org. Chem. 1993, 58, 7310.