Supporting Information

Kinetics and Mechanism of the Pyridinolysis of Diisopropyl Chlorothiophosphate in Acetonitrile

Md. Ehtesham Ul Hoque and Hai Whang Lee*

*Department of Chemistry, Inha University, Incheon 402-751, Korea. *E-mail: hwlee@inha.ac.kr*
Received April 25, 2012, Accepted July 2, 2012

Product : $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$

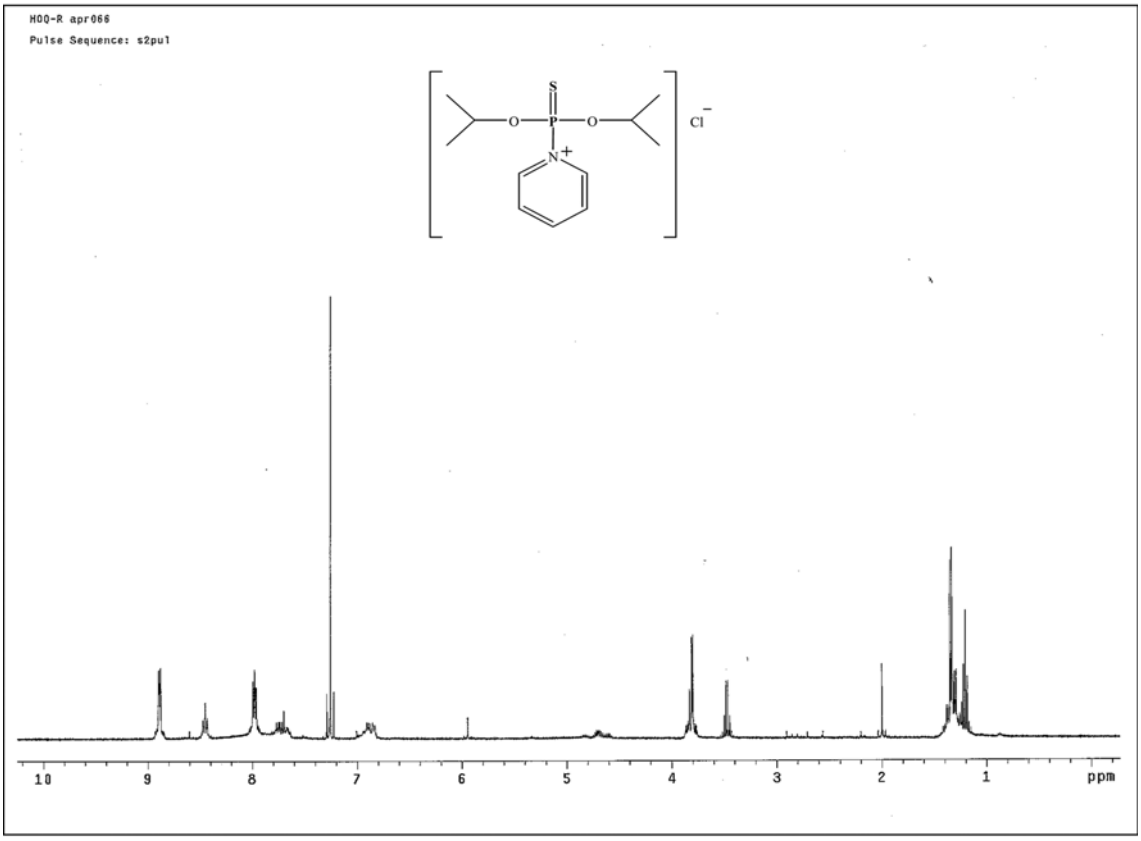

Figure S1. The ^{1}H-NMR spectrum of $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$.

Product : $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$

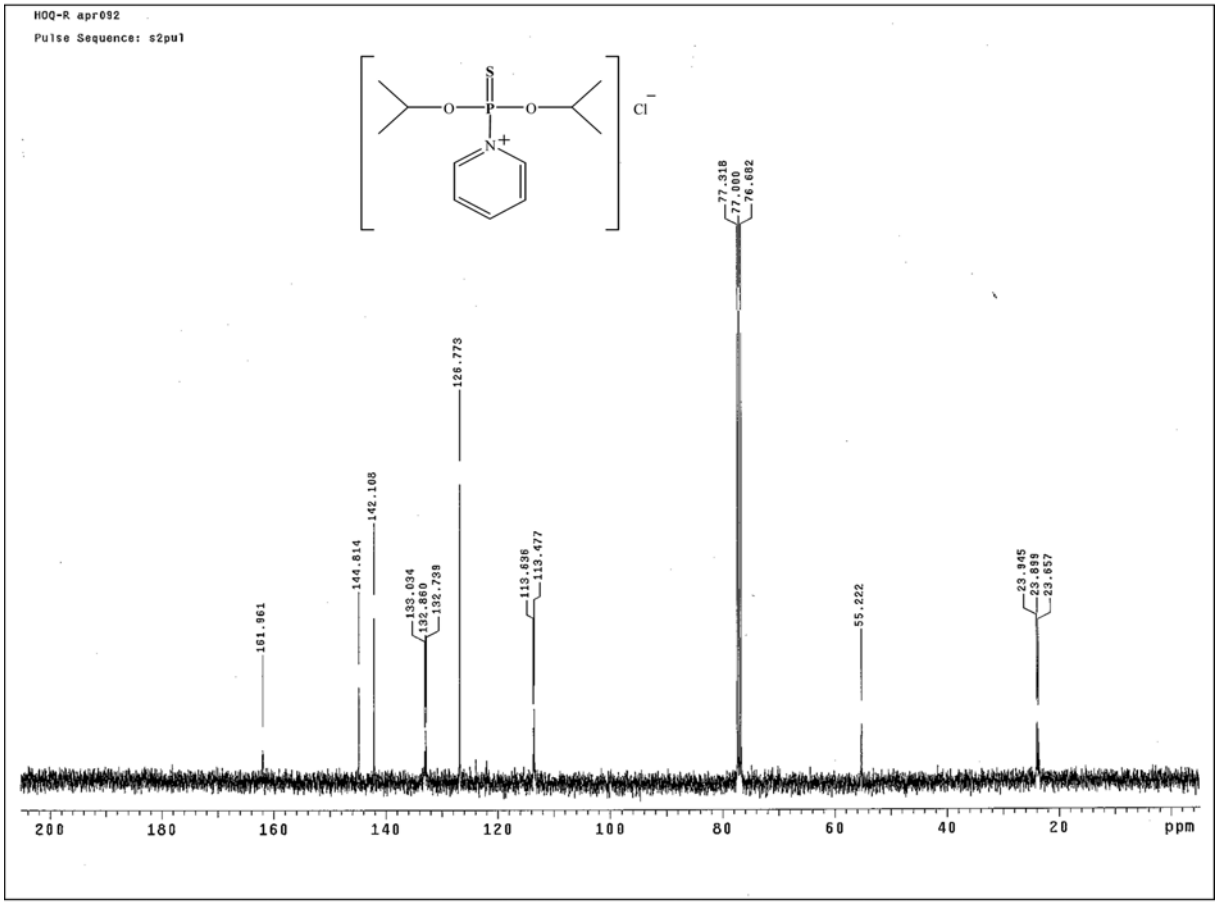

Figure S2. The ^{13}C-NMR spectrum of $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$.

Product : $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$

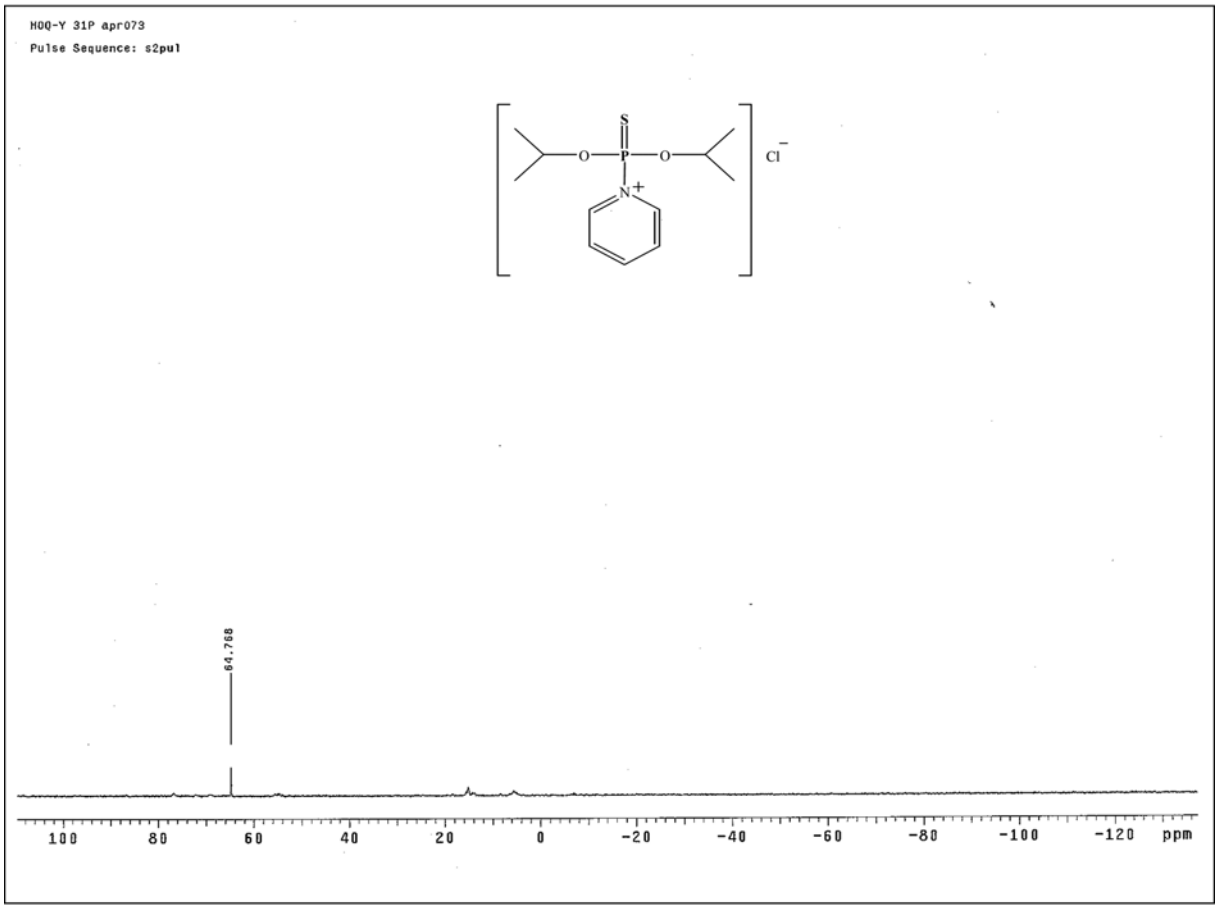

Figure S3. The ^{31}P-NMR spectrum of $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$.

Product : $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$

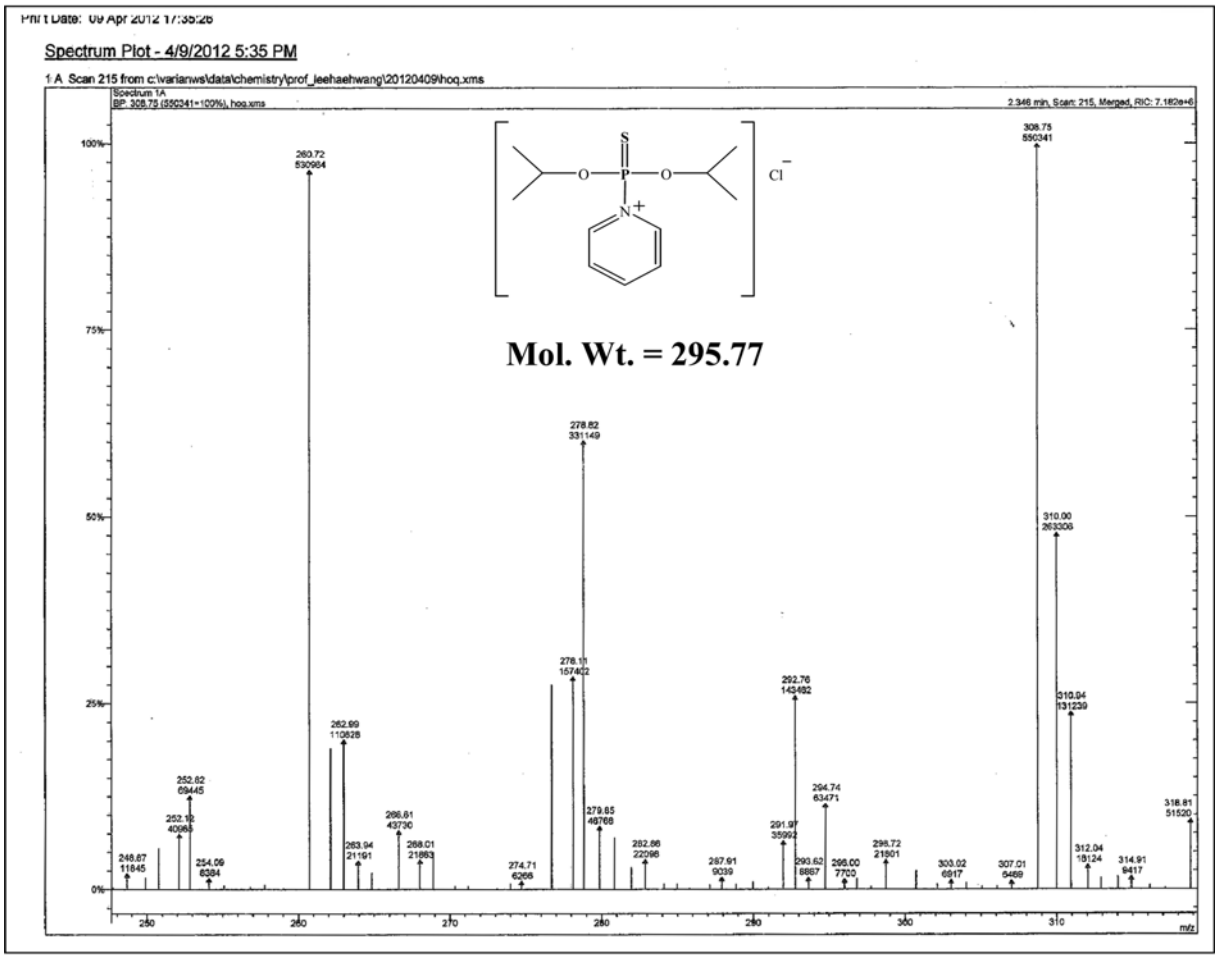

Figure S4. The LC-MS spectrum of $[(i\text{-PrO})_2P(=S)NC_5H_5]^+Cl^-$.

Activation Parameters

Table S1. Activation Parameters[a] for the Reaction of Diisopropyl Chlorothiophosphate with C_5H_5N in MeCN

t / ℃	$k_2 \times 10^4$ /M^{-1} s^{-1}	$\Delta H^{\neq}$/kcal mol^{-1}	$-\Delta S^{\neq}$/cal mol^{-1} K^{-1}
35.0	4.60 ± 0.02		
40.0	7.00 ± 0.03	15.2 ± 0.4[b]	25 ± 1[c]
45.0	10.6 ± 0.1		

[a]Calculated by the Eyring equation. [b,c]Standard deviation.

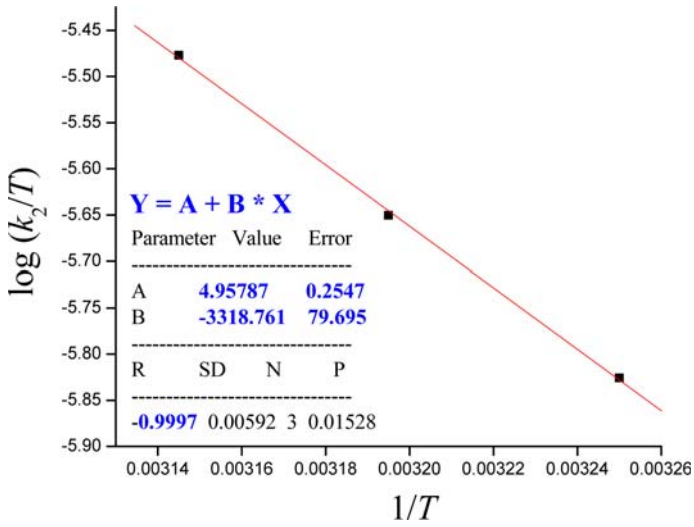

Figure S5. A plot of log (k_2/T) *vs*. 1/T for the reaction of diisopropyl chlorothiophosphate with pyridine in MeCN.