

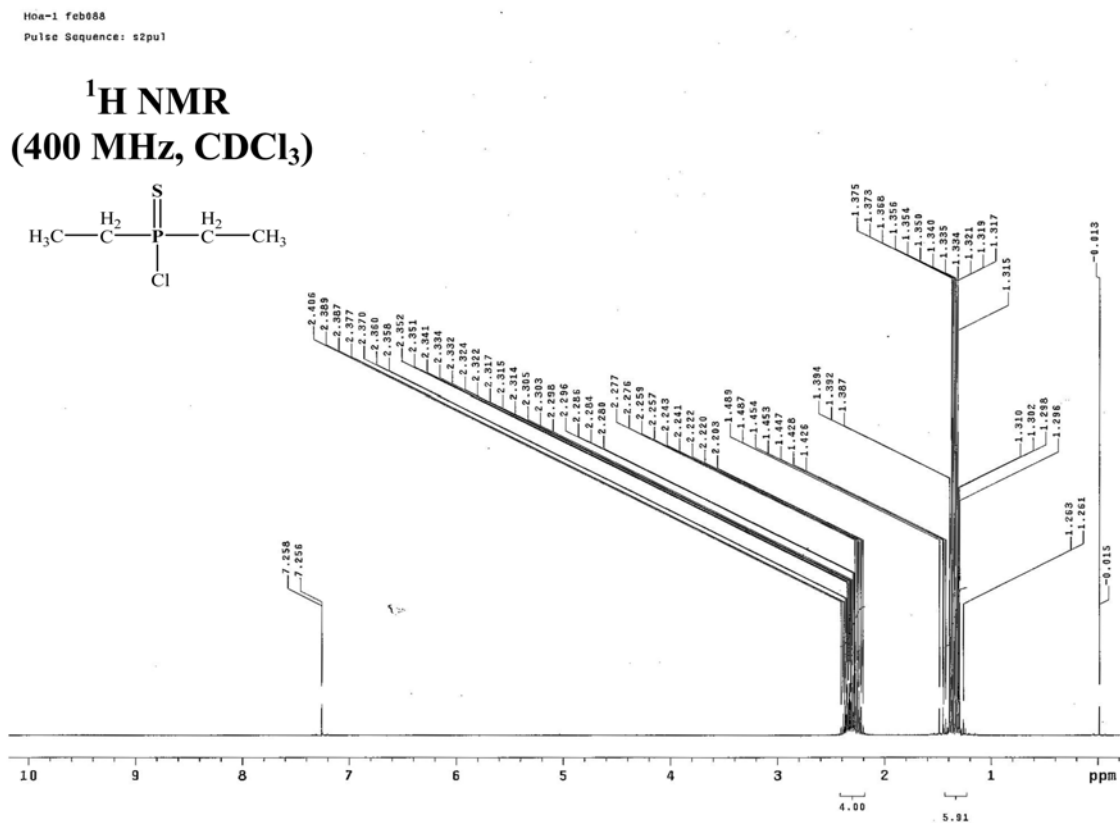
Supplementary Materials

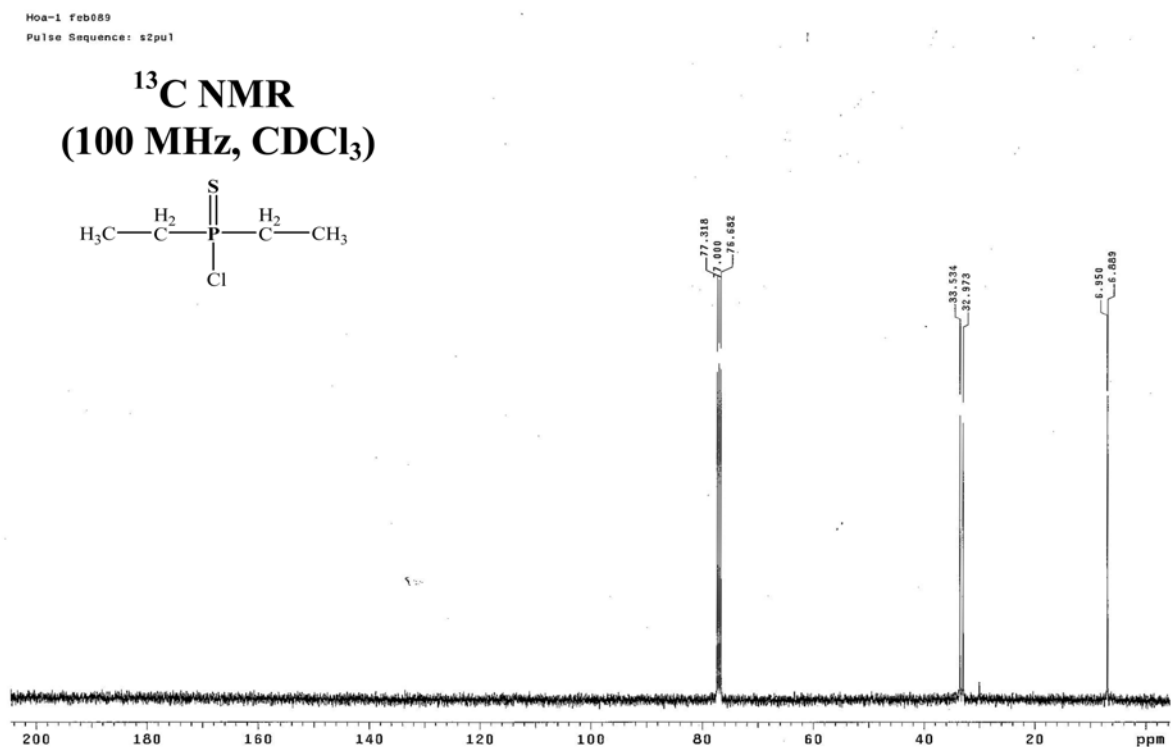
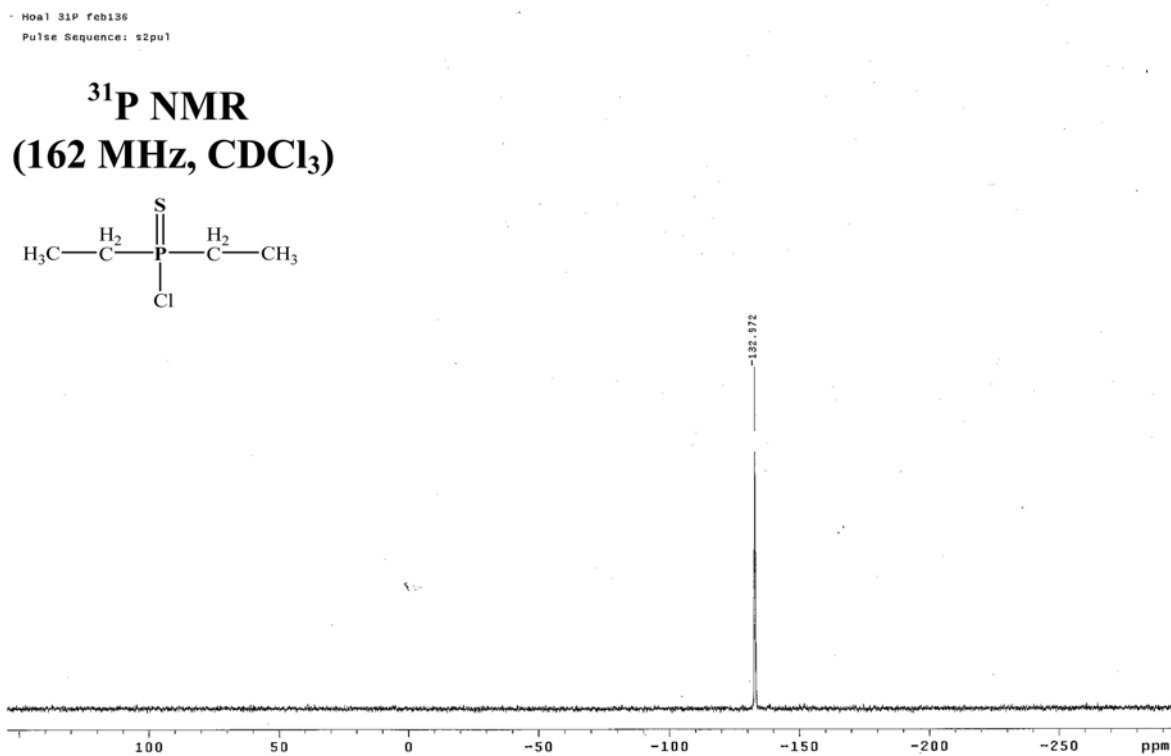
Kinetics and Mechanism of the Anilinolysis of Diethyl Thiophosphinic Chloride in Acetonitrile

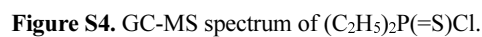
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Received May 13, 2011, Accepted May 24, 2011**Table 1.** Activation Parameters^a for the Reactions of Diethyl Thiophosphinic Chloride with XC₆H₄NH₂ in MeCN at 55.0 °C

X	Temp. / °C	$k_H \times 10^4$ /M ⁻¹ s ⁻¹	ΔH^\ddagger /kcal mol ⁻¹	$-\Delta S^\ddagger$ /cal mol ⁻¹ K ⁻¹
	45	2.32 ± 0.02		
H	55	3.30 ± 0.03	7.1 ± 0.3 ^b	53 ± 1 ^c
	65	4.80 ± 0.04		

^a Calculated by Eyring equation. ^{b,c} Standard deviation.Substrate; (C₂H₅)₂P(=S)Cl:**Figure S1.** ¹H NMR spectrum of (C₂H₅)₂P(=S)Cl.

**Figure S2.** ^{13}C NMR spectrum of $(\text{C}_2\text{H}_5)_2\text{P}(=\text{S})\text{Cl}$.**Figure S3.** ^{31}P NMR spectrum of $(\text{C}_2\text{H}_5)_2\text{P}(=\text{S})\text{Cl}$.



¹H NMR
(400 MHz, CDCl₃)

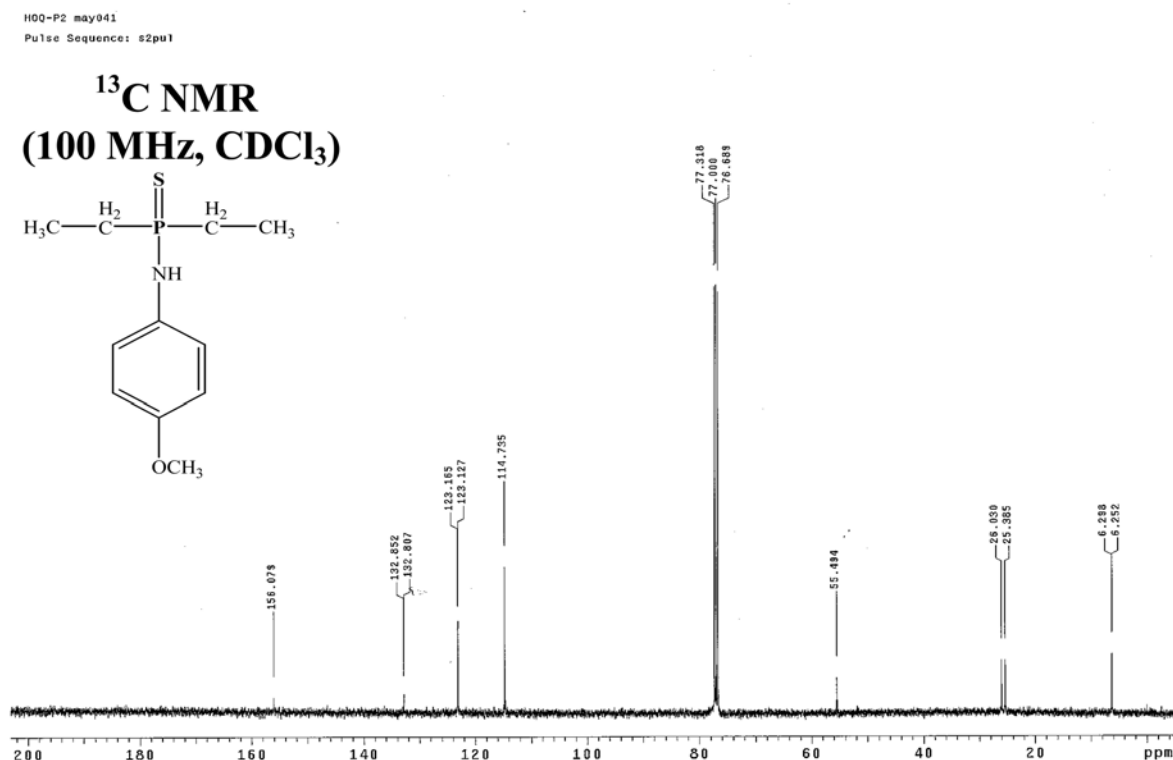
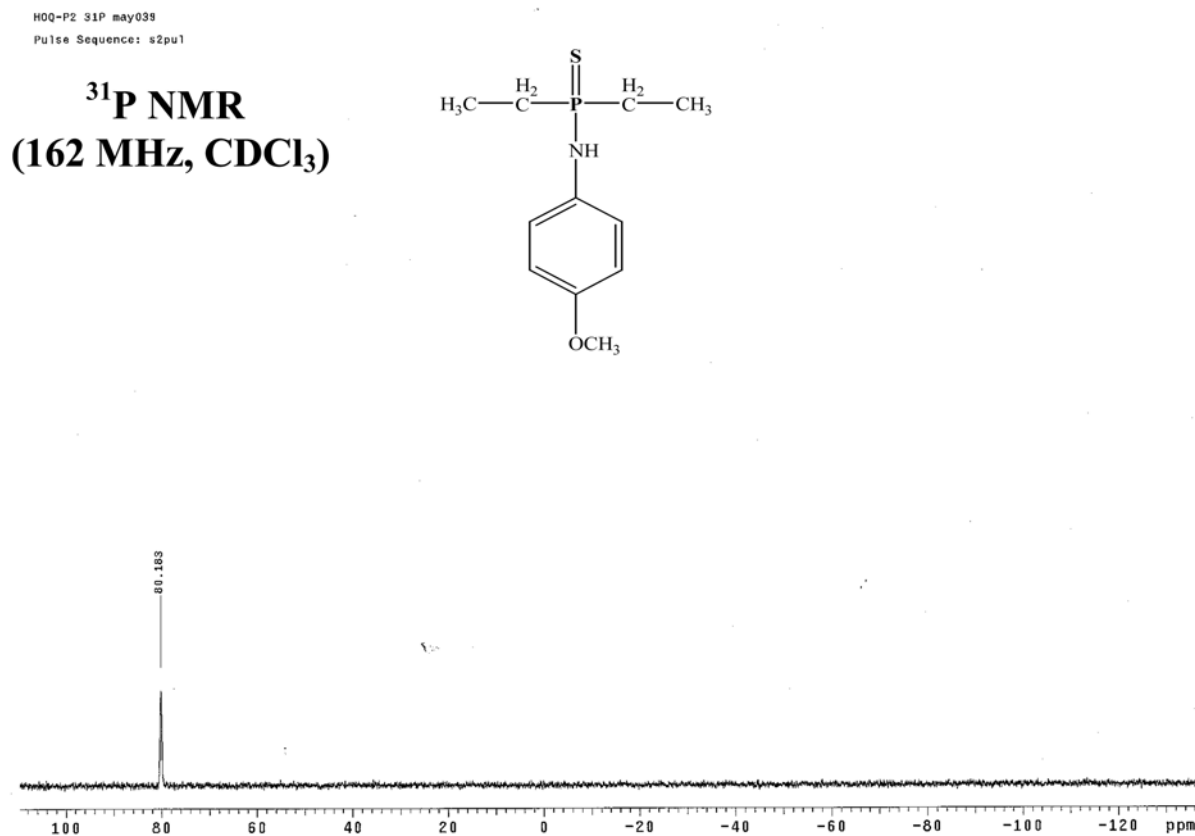
CCOP(=S)(CC)Cc1ccc(OC)cc1

Chemical structure of 1-(4-methoxyphenyl)propyl phosphorothioate is shown above the spectrum. The structure is: CCOP(=S)(CC)Cc1ccc(OC)cc1.

The spectrum displays the following chemical shifts (ppm) and integrations:

- ~7.2 ppm (s, 2H, integration 2.22)
- ~6.8 ppm (d, 2H, integration 2.08)
- ~3.8 ppm (s, 3H, integration 3.00)
- ~3.7 ppm (q, 2H, integration 0.94)
- ~3.4 ppm (d, 1H, integration 3.00)
- ~2.0 ppm (m, 2H, integration 4.34)
- ~1.2 ppm (m, 3H, integration 6.29)
- ~0.0 ppm (s, 3H, integration 0.006)

Figure S5. ^1H NMR spectrum of $(\text{C}_2\text{H}_5)_2\text{P}(=\text{S})\text{NH}-\text{C}_6\text{H}_4-4-\text{CH}_3\text{O}$.

**Figure S6.** ^{13}C NMR spectrum of $(\text{C}_2\text{H}_5)_2\text{P}(=\text{S})\text{NH}-\text{C}_6\text{H}_4-4-\text{CH}_3\text{O}$.**Figure S7.** ^{31}P NMR spectrum of $(\text{C}_2\text{H}_5)_2\text{P}(=\text{S})\text{NH}-\text{C}_6\text{H}_4-4-\text{CH}_3\text{O}$.

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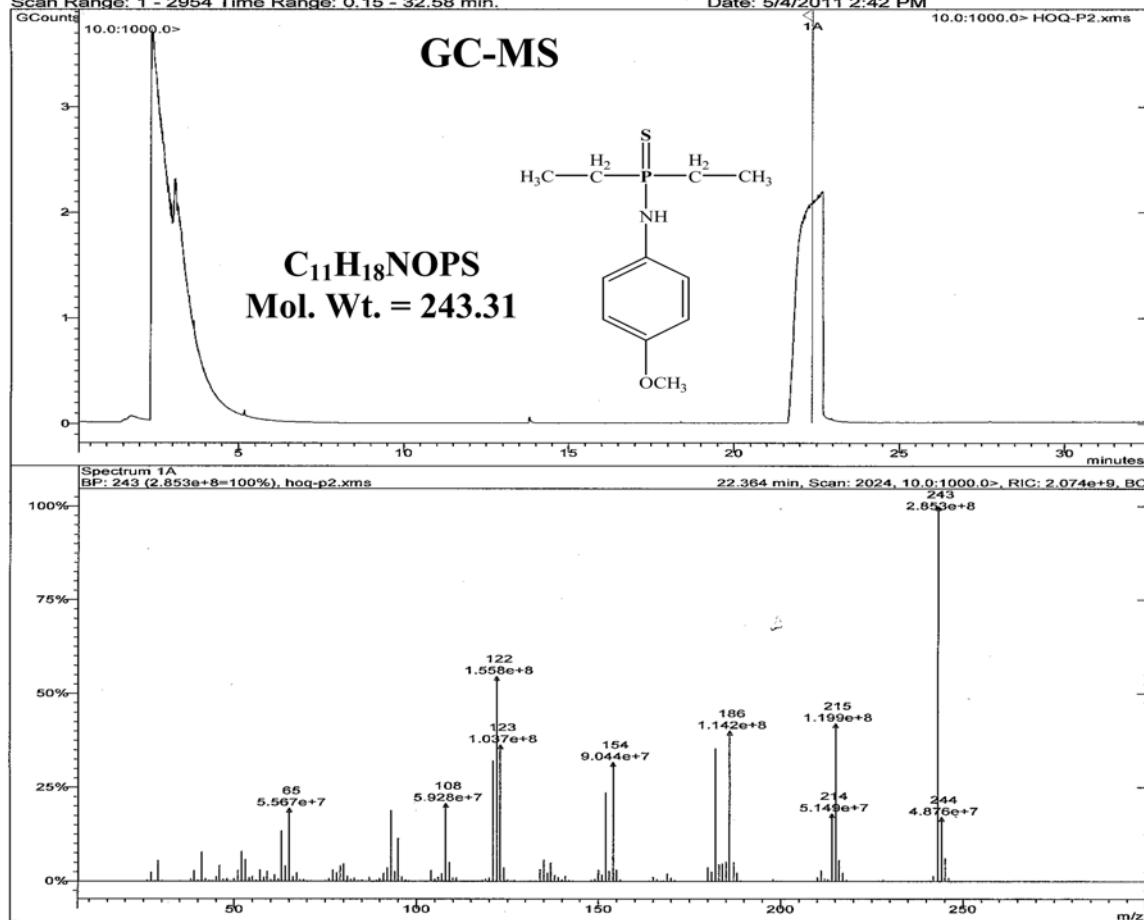
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Figure S8. GC-MS spectrum of $(C_2H_5)_2P(=S)NH-C_6H_4-4-CH_3O$.