

10.1071/CH16202\_AC

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Australian Journal of Chemistry 70(1), 101-105

## SUPPLEMENTARY MATERIAL

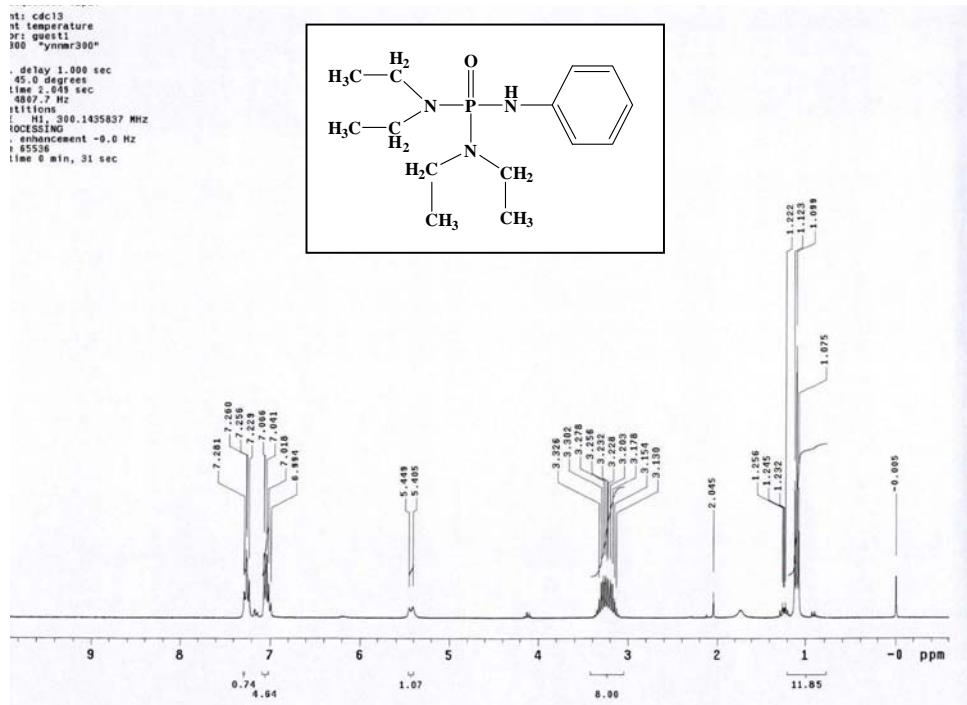
### **Concerted Pathway to Mechanism of Anilinolysis of Bis(*N,N*-diethylamino)phosphinic Chloride in Acetonitrile**

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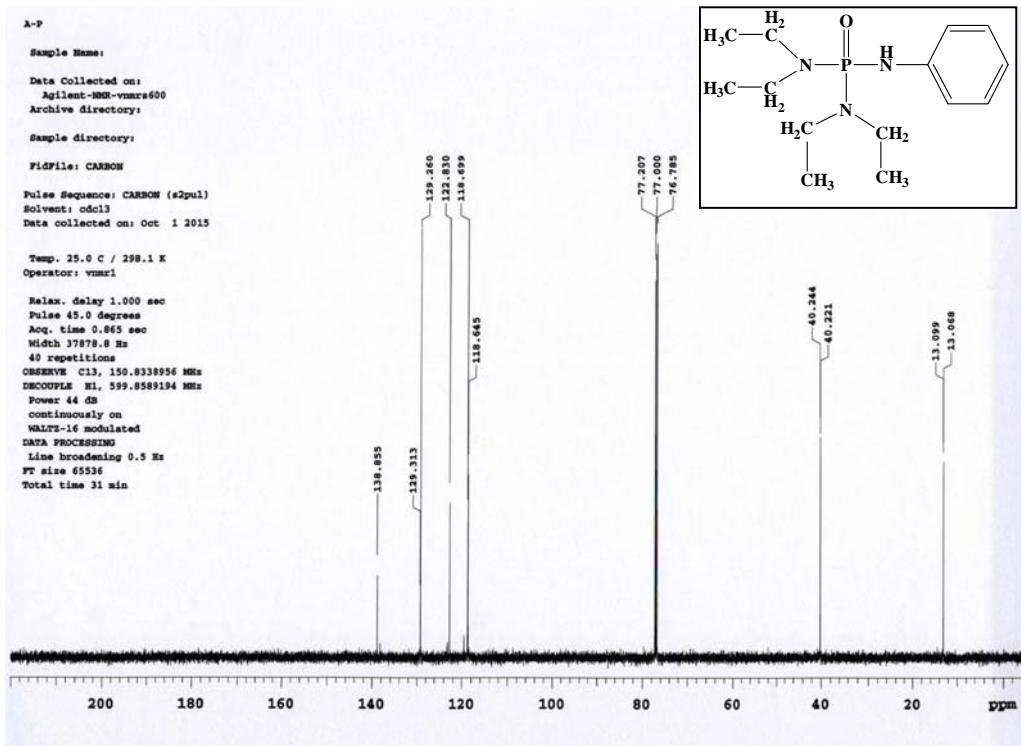
Email: [hrbarai@ynu.ac.kr](mailto:hrbarai@ynu.ac.kr)      Contact: Tel: (82) 053 810 3547

**Product:  $[C_8H_{20}N_2P(=O)NHC_6H_5]$**



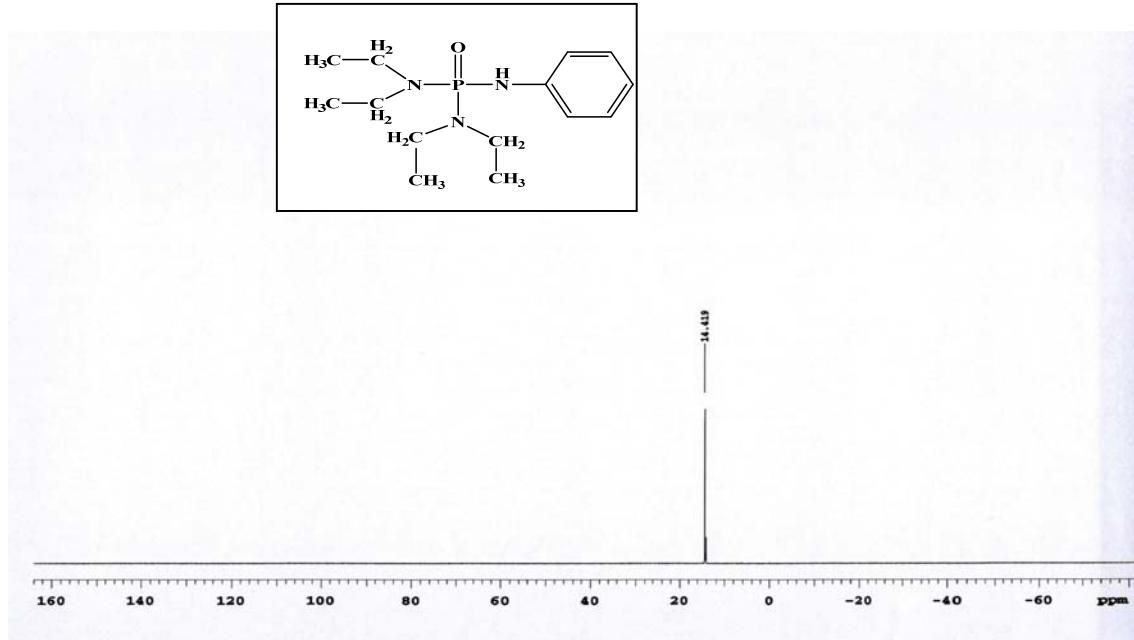
**Figure S1.** The  $^1\text{H}$ -NMR spectrum of  $[C_8H_{20}N_2P(=O)NHC_6H_5]$ .

**Product:  $[C_8H_{20}N_2P(=O)NHC_6H_5]$**



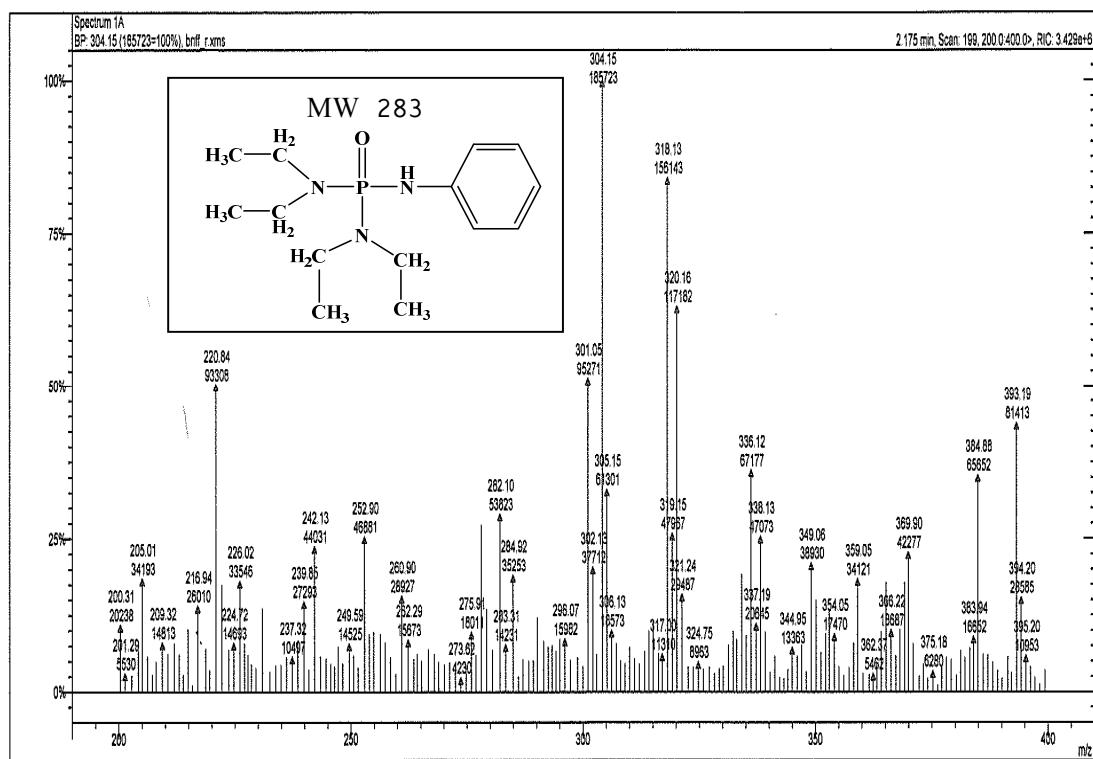
**Figure S2.** The  $^{13}\text{C}$ -NMR spectrum of  $[C_8H_{20}N_2P(=O)NHC_6H_5]$ .

**Product:**  $[C_8H_{20}N_2P(=O)NHC_6H_5]$



**Figure S3.** The  $^{31}P$ -NMR spectrum of  $[C_8H_{20}N_2P(=O)NHC_6H_5]$ .

**Product:  $[C_8H_{20}N_2P(=O)NHC_6H_5]$**



**Figure S4.** The LC-MS spectrum of  $[C_8H_{20}N_2P(=O)NHC_6H_5]$ .

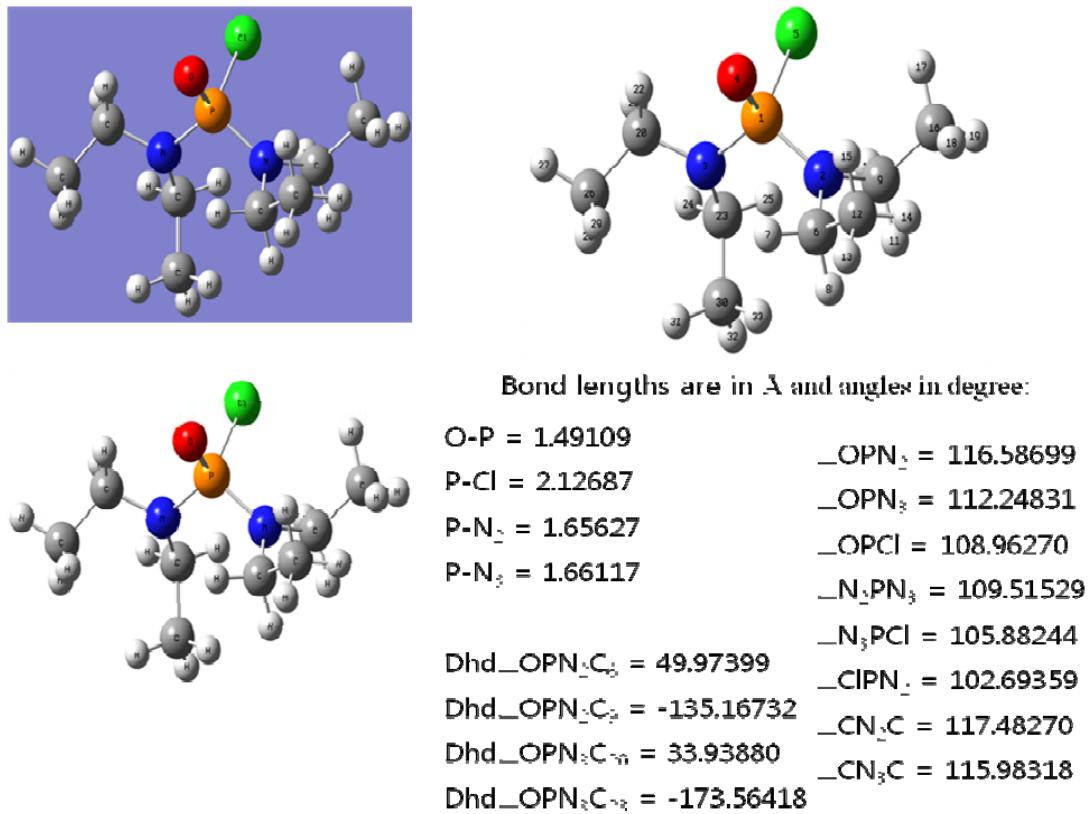


Figure S5. The geometry of bis(*N,N*-diethylamino)phosphinic chloride (**4**) in the gas phase calculation by Gaussian 09 Program, B3LYP Level of Theory 6-311+G(d,p) Basis set, CPCM method, acetonitrile continuum model.

**Table S1.** The geometry of bis(*N,N*-diethylamino)phosphinic chloride (**4**) in the gas phase by Gaussian 09 Program, B3LYP Level of Theory 6-311+G(d,p) Basis set.

## Summary of Natural Population Analysis:

Natural Population						
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
P	1	2.19346	9.99776	2.67459	0.13419	12.80654
N	2	-0.90650	1.99938	5.87653	0.03059	7.90650
N	3	-0.88326	1.99938	5.85175	0.03213	7.88326
O	4	-1.09787	1.99982	7.08755	0.01050	9.09787
Cl	5	-0.35267	9.99979	7.34144	0.01144	17.35267
C	6	-0.16782	1.99928	4.14945	0.01908	6.16782
H	7	0.20569	0.00000	0.79163	0.00268	0.79431
H	8	0.19719	0.00000	0.80094	0.00187	0.80281
C	9	-0.16864	1.99928	4.15037	0.01899	6.16864
H	10	0.20395	0.00000	0.79401	0.00204	0.79605
H	11	0.20221	0.00000	0.79601	0.00178	0.79779
C	12	-0.58673	1.99936	4.57897	0.00841	6.58673
H	13	0.20934	0.00000	0.78931	0.00135	0.79066
H	14	0.20013	0.00000	0.79816	0.00170	0.79987
H	15	0.20646	0.00000	0.79178	0.00176	0.79354
C	16	-0.58649	1.99935	4.57902	0.00812	6.58649
H	17	0.20544	0.00000	0.79275	0.00181	0.79456
H	18	0.20036	0.00000	0.79785	0.00179	0.79964
H	19	0.20688	0.00000	0.79173	0.00139	0.79312
C	20	-0.17025	1.99929	4.15325	0.01771	6.17025
H	21	0.18702	0.00000	0.81087	0.00211	0.81298
H	22	0.21692	0.00000	0.78093	0.00215	0.78308
C	23	-0.17740	1.99929	4.15927	0.01884	6.17740
H	24	0.20290	0.00000	0.79528	0.00181	0.79710
H	25	0.20032	0.00000	0.79770	0.00198	0.79968
C	26	-0.58655	1.99936	4.57834	0.00886	6.58655
H	27	0.21099	0.00000	0.78772	0.00129	0.78901
H	28	0.20014	0.00000	0.79819	0.00167	0.79986
H	29	0.20398	0.00000	0.79419	0.00183	0.79602
C	30	-0.58201	1.99935	4.57382	0.00884	6.58201
H	31	0.20337	0.00000	0.79499	0.00164	0.79663
H	32	0.20767	0.00000	0.79101	0.00132	0.79233
H	33	0.20175	0.00000	0.79662	0.00162	0.79825
* Total *		0.00000	41.99070	79.64602	0.36328	122.00000
Natural Population						
Core			41.99070	( 99.9779% of 42)		
Valence			79.64602	( 99.5575% of 80)		
Natural Minimal Basis			121.63672	( 99.7022% of 122)		
Natural Rydberg Basis			0.36328	( 0.2978% of 122)		

**Table S2.** Activation parameters for the reactions of bis(*N,N*-diethylamino)phosphinic chloride with anilines in acetonitrile.

$t/^\circ\text{C}$	$k_{\text{H}} \times 10^5 / \text{M}^{-1} \text{s}^{-1}$	$\Delta H^\ddagger / \text{kcal.mol}^{-1}$	$-\Delta S^\ddagger / \text{cal.mol}^{-1} \cdot \text{K}^{-1}$
45	$1.59 \pm 0.01$		
55	$2.97 \pm 0.01$	11.9	43
65	$5.16 \pm 0.01$		