Heteroatom Chemistry
Volume 10, Number 7, 1999

1,3-Azaphospholo[5,1-*a*]isoquinolines

Raj K. Bansal, Leena Hemrajani, and Neelima Gupta

Department of Chemistry, University of Rajasthan, Jaipur 302 004, India.

Received: 11 June 1999

ABSTRACT: *In a one pot synthesis, 1,3-azaphospholo[5,1-a]isoquinoline (***4***) was obtained from the reaction of N-(alkoxycarbonylmethyl)isoquinolinium bromide (***1***) with* PCl_3 *in the presence of* $(C_2H_5)_3N$*. A crossed reaction confirms the formation of* **4** *proceeding via a 1,5-electrocyclization. Compound* **4** *undergoes [2 + 4] cycloaddition with 2,3-dimethyl-1,3-butadiene in the presence of sulfur. The influence of the substituent group on the reactivity of the C = P– moiety in the 1,3-azaphospholo ring toward [2 + 4] cycloaddition is corroborated by semiempirical PM3 calculations.* © 1999 John Wiley & Sons, Inc. Heteroatom Chem 10: 598–604, 1999

INTRODUCTION

The annulated azaphospholes represent interesting heteroaromatic systems with σ^2,λ^3-phosphorus, which incorporates several functionalities [1,2]. The 1,3-azaphospholo[1,5-*a*]pyridines, which are named as 2-phosphaindolizines, became first accessible through the [4 + 1] cyclocondensation of 1,2-dialkylpyridinium bromides with phosphorus trichloride in the presence of triethylamine [3–5]. Later, they were also obtained from the [3 + 2] cycloaddition of the *N*-pyridinium ylides, generated in situ, with phosphaalkynes [6]. Recently, we developed another synthetic method for these compounds involving disproportionation of the *N*-pyridinium dichlorophosphinomethylides, followed by 1,5-electrocyclization [7]. In view of the similar behavior shown by the *N*-pyridinium ylides with *N*-isoquinolinium ylides [8], the method of 1,5-electrocyclization is now extended to the synthesis of 1,3-bis(alkoxycarbonyl)[1,3]azaphospholo[5,1-*a*]isoquinolines, which we report in this paper. The 1,3-azaphospholo[5,1-*a*]isoquinolines were earlier prepared from the [3 + 2] cycloaddition of the *N*-isoquinolinium ylides with phosphaalkynes [9].

In azaphospholes, the two-coordinate phosphorus represents the main center of reactivity. A large number of 1,2-addition reactions of various reagents across the P = C or P = N double bond have been reported for electron-poor azaphospholes [1,10–12]. These additions may or may not be accompanied by an oxidation of the phosphorus atom. Although 3-ethoxycarbonyl-2-phosphaindolizine was found to be unreactive toward 2,3-dimethyl-1,3-butadiene (Bansal and Gupta, unpublished observations), 1,3-bis(ethoxycarbonyl)-2-phosphaindolizine reacted under these conditions (Bansal, et al., unpublished observations). Likewise, 1,3-bis(ethoxycarbonyl)[1,3]azaphospholo[5,1-*a*]isoquinoline undergoes [2 + 4] cycloaddition with 2,3-dimethyl-1,3-butadiene in the presence of sulfur. The results are described here. The relative reactivities of mono- and disubstituted 2-phosphaindolizines and 1,3-azaphospholo[5,1-*a*]isoquinoline have been explained on the basis of semiempirical PM3 (Pennsylvanian Model 3) calculations.

RESULTS AND DISCUSSION

Synthesis of 1,3-Azaphospholo[5,1-a]isoquinolines

N-Alkoxycarbonylmethylisoquinolinium bromides **1a–c** react with one equivalent of PCl_3 and two equivalents of triethylamine at ambient temperature in

Correspondence to: Raj K. Bansal
Contract Grant Sponsor: B. R. N. S., Department of Atomic Energy, Government of India.
Dedicated to Prof. Dr. Alfred Schmidpeter on the occasion of his 70th birthday.
 CCC 1042-7163/99/070598-07

toluene to form *N*-isoquinolinium alkoxycarbonyl, dichlorophosphinomethylides **2a–c,** as indicated by the appearance of a ^{31}P-NMR signal at $\delta \sim 150$ [7,13]. However, in contrast to *N*-pyridinium dichlorophosphinomethylides [13], these compounds (**2a–c**) could not be isolated in the pure state, as during workup, **2a** and **2b** changed into 1,3-azaphospholo[5,1-*a*]isoquinolines **4a** and **4b** respectively, whereas no cyclization product was obtained from **2c.** The reaction of **1d** under these conditions is not clean, and a dark-colored insoluble material is formed.

As in the case of *N*-pyridinium dichlorophosphinomethylides [7], the initially formed *N*-isoquinolinium alkoxycarbonyl, dichlorophosphinomethylides **2a,b** are expected to undergo disproportionation to generate bis(*N*-isoquinolinium ylidyl)phosphenium chlorides **3,** which by virtue of incorporating a 1,5-dipolar structure, undergo 1,5-electrocyclization [14] followed by loss of the isoquinolinium chloride to form **4a,b** (Scheme 1).

In a one-pot synthesis, **4** is prepared from the reaction of **1** with PCl_3 (0.5 equiv.) in the presence of triethylamine (2 equiv.) in a polar solvent like methylene chloride (Scheme 2).

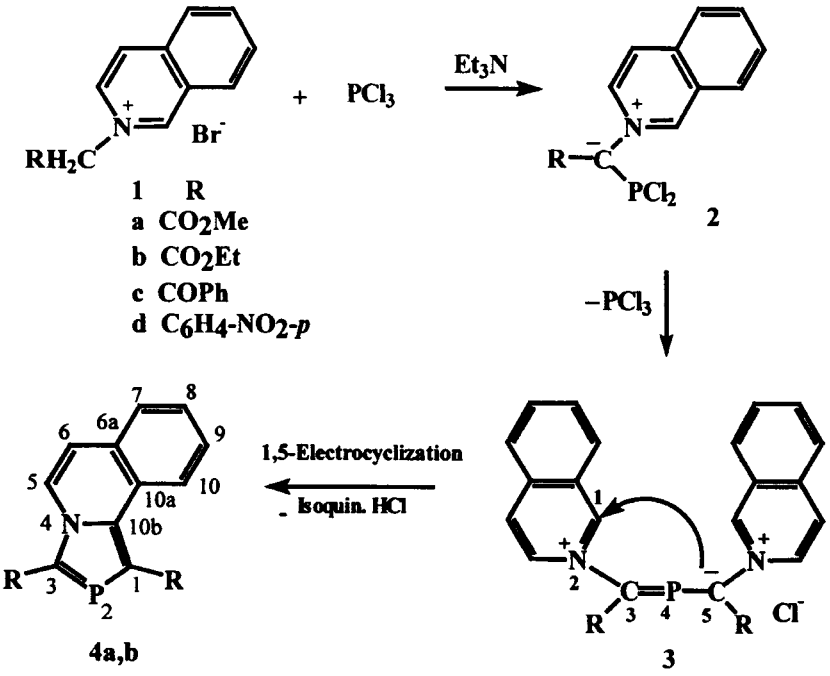
The product obtained by performing a crossed reaction between **1b** and **2a** under similar conditions is found to be a mixture of four compounds **4a, 4b, 5,** and **6,** (Scheme 3) as indicated by ^{31}P- and ^{1}H-NMR data (Table 1). Although only three ^{31}P-NMR signals are observed at δ = 175.25, 175.36, and 175.40, appearance of the four most downfield doublets in the ^{1}H-NMR spectrum at δ = 9.62, 9.63, 9.67, and 9.68, which correspond to the 5-H proton, confirms the presence of four compounds in the mixture. This conclusion is further supported by the presence of four sets of triplets and quartets for the ethoxy groups and four singlets for the methoxy groups. It is possible that the expected fourth ^{31}P-NMR signal is not resolved or that two compounds have an identical ^{31}P-NMR chemical shift.

The formation of **5** and **6** confirms the intermediacy of **3.** The compounds **4a** and **4b** are yellow solids, soluble in common organic solvents such as acetonitrile, methylene chloride, and chloroform.

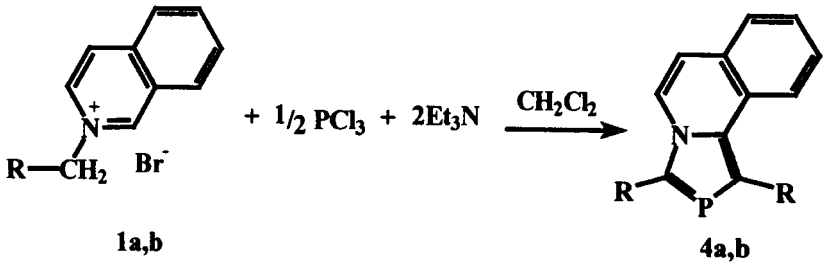
NMR Data

The structures of 1,3-azaphospholo[5,1-*a*]isoquinolines **4a,b** have been elucidated by ^{31}P-, ^{1}H-, and ^{13}C-NMR data (Tables 1 and 2).

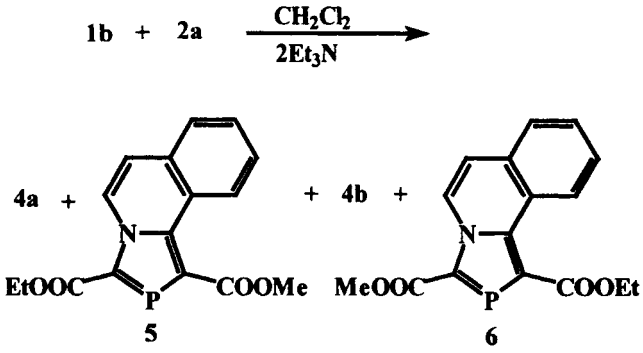
The ^{31}P-NMR chemical shift of **4** at $\delta \sim 174$ is in the range characteristic for 1,5-annulated-1,3-azaphospholes [1,3–7,11,15] and quite close to that of the analogous 1,3-azaphospholo[1,5-*a*]pyridines having two alkoxycarbonyl substituents on carbons adjacent to the σ^2,λ^3 phosphorus [7]. The most deshielded signal in the ^{1}H-NMR spectrum of **4a,b** is a doublet at δ = 9.4–9.6 corresponding to the 5-H. On the other hand, 6-H ($\delta \sim 7.1$) is the most shielded



SCHEME 1



SCHEME 2



SCHEME 3

aromatic proton. 10-H appears as a doublet of double doublets at δ = 8.9 in **4b.** The 7-H, 8-H, and 9-H give multiplets in the region δ = 7.5–7.7.

In the ^{13}C-NMR spectrum of **4b,** assignment of signals has been made on the basis of long range C-P coupling constants [1,16]. The characteristic features in the ^{13}C NMR spectrum of **4b** are the doublets at δ = 134.5 and 142.9, with ^{1}J(P,C) coupling constants of 44.4 and 47.9 Hz, respectively. Since C-3 has a formal double bond with phosphorus, it is expected to have a larger coupling constant than C-1. Thus, the doublet at δ = 142.9 is assigned to C-3, and the doublet at δ = 134.5 is assigned to C-1. The chemical shift values of the other carbons compare well with those reported for 1-*tert*-butyl-3-methoxycarbonyl[1,3]-azaphospholo[1,5-*a*]isoquinoline [9].

Mass Spectral Fragmentation of **4b**

The mass spectral fragmentation of **4b** only partly resembles that of 2-phosphaindolizines [5]. In contrast to 2-phosphaindolizines, the molecular ion of **4b** forms the base peak in the spectrum. The preliminary fragmentation is initiated at the –P=C–COOEt part of the molecule as shown in Scheme 4. The characteristic feature is the loss of P≡C–COOEt from the molecular ion to form an ion **B** at *m/z* 213. Formation of the latter can be stipulated through another route involving successive loss of an ethoxy radical, a CO molecule, and HC≡P. Furthermore, B subsequently rearranges to C, which leads to the formation of other prominent ions observed in the spectrum. Alternatively, B may generate the isoquinolinium ion, which gives other ions that are typically observed in the mass spectrum of isoquinolines [17].

PM3 Calculations and [2+4] Cycloaddition

The feasibility of [2+4] cycloaddition and the reactivities of the 1,3-diene and dienophile were correlated earlier with the energy gap between the frontier orbitals of the reactants [18–20]. It was demonstrated on the basis of semiempirical calculations that the nature of the substituent groups affects the energy levels of the frontier orbitals and hence the reactivity of the dienophile [18,19]. The C=P moiety in the azaphospholes acts as a dienophile [1,11] and the nature of the substitution on its two ends was found to affect its reactivity. 3-Ethoxycarbonyl-2-phosphaindolizine was found to be unreactive toward 2,3-dimethyl-1,3-butadiene even with prolonged heating in toluene, whereas 1,3-bis(ethoxycarbonyl)-2-phosphaindolizine reacted under these condition to form a [2+4] cycloadduct (Bansal et al., unpublished results). To explain this difference in reactivity, the energies of the frontier orbitals of the mono- and disubstituted as well as unsubstituted 2-phosphaindolizines and 1,3-azaphospholo[5,1-*a*]isoquinolines were obtained by semiempirical PM3 calculations, which are shown in Figure 1. In each case the energy gap, $HOMO_{diene} - LUMO_{dienophile}$ being smaller, the reaction is $LUMO_{dienophile}$ controlled. This energy difference in the case of monosubstituted 2-phosphaindolizine and 1,3-azaphospholo[5,1-*a*]isoquinoline being still greater than 8.0 eV explains the inertness of these dienophiles in [2+4] cycloaddition. Introduction of an additional ethoxycarbonyl group in the 1-position causes lowering of the $HOMO_{diene} - LUMO_{dienophile}$ energy gap below 8.0 eV, thereby making [2+4] cycloaddition feasible.

As expected from these results, 1,3-bis(eth-

TABLE 1 ^{31}P NMR and ^{1}H NMR Data of 1,3-Azaphospholo[5,1-*a*]isoquinolines and [2 + 4] cycloadduct **7**[a,b]

δJ (Hz)	**4a**	**4b**	**4a** + **4b** + **5** + **6**	**7**[c]
^{31}P	173.24	174.53	175.25, 175.36, 175.40	68.2
5-H	9.57	9.64	9.62, 9.63, 9.67, 9.68	8.93
^{3}J (5H,6H)	7.8	7.7	7.7, 7.6, 7.7, 7.6	8.3
6-H	7.12	7.16	6.47, 6.49	6.63
^{3}J (6H,5H)	7.8	7.7	7.7, 7.6	7.3
7-H, 8-H, 9-H	7.37–7.93	7.57–7.70	7.00–7.30	7.49[d], 7.64
^{3}J (H,H)				7.6, 7.3
^{4}J (H,H)				1.4, 1.3
10-H	9.17	8.90	9.20–9.39	7.47
^{3}J (10H,9H)	8.3	7.1		7.6
^{4}J (10H,8H)		3.0		
^{5}J (10H,7H)		0.7		
1-, 3-OCH_3	3.87, 3.92		3.49, 3.50, 3.61, 3.62	
1-, 3-OCH_2		4.40, 4.46	4.14, 4.15, 4.20, 4.26	4.25–4.36
CH_3		1.42, 1.45	1.06, 1.08, 1.14, 1.15	1.27, 1.41
^{3}J (H,H)		7.1	7.1	7.1

[a] **4a, 4b,** and **7** in $CDCl_3$ and mixture (**4a** + **4b** + **5** + **6**) in C_6D_6.
[b] **4a** on JEOL FX 90Q, **4b** on JEOL EX 400, and mixture (**4a** + **4b** + **5** + **6**) and **7** on Bruker ARX 300.
[c] 11-CH_2 {$H_A\delta$3.48, $H_B\delta$3.48, ^{2}J (H_AH_B) = 15.5 Hz, ^{2}J (H_AP) = 15.5 Hz, ^{2}J (H_BP) = 13.7 Hz}; 14-CH_2 {$H_A\delta$2.98, $H_B\delta$2.82, ^{2}J (H_AH_B) = 15.5 Hz, ^{3}J (H_AP) = 16.5 Hz, ^{3}J (H_BP) = 23.0 Hz}; 12-$CH_3\delta$1.53, ^{4}J (PH) = 5.9 Hz; 13-$CH_3\delta$ 1.67.
[d] 7-H δ6.92, ^{3}J (HH) = 7.3 Hz.

TABLE 2 ^{13}C-NMR Data of 1,3-Bis(ethoxycarbonyl)[1,3] azaphospholo[5,1-*a*]isoquinoline **4b** and [2 + 4] Cycloadduct **7**($CDCl_3$)

δ *J* (Hz)	**4b**	**7**[a]
C-1	134.5	81.6
^{1}J (P,C)	44.4	83.3
C-3	142.9	72.3
^{1}J (P,C)	47.9	54.7
C-5	129.6	132.3
C-6	115.6	109.7
^{4}J (P,C)	2.3	
C-6a	123.9	121.7
^{4}J (P,C)	2.3	10.5
C-7, C-8, C-9	127.8, 127.5, 126.6	125.8, 125.7, 125.2
C-10	129.4	131.0
^{4}J (P,C)	1.3	
C-10a	125.6	125.6
^{3}J (P,C)	3.3	
C-10b	142.5	134.5
^{2}J (P,C)	7.7	<1
1-OCH_2	61.5, 61.1	62.1
3-OCH_2		59.2
$OCH_2\underline{C}H_3$	14.4	13.5, 13.3
1-CO	163.3	164.4
^{2}J (P,C)	19.4	9.8
3-CO	167.8	159.3
^{2}J (P,C)	20.6	9.1

[a] C-11 δ39.4, ^{1}J (P,C) = 51.3 Hz; C-12 δ125.0, ^{2}J (P,C) = 12.8 Hz; C-13 δ126.5, ^{3}J (P,C) = 5.3 Hz; C-14 δ38.8; 12-CH_3 δ19.2, ^{3}J (P,C) = 4.2 Hz; 13-CH_3 δ 19.1.

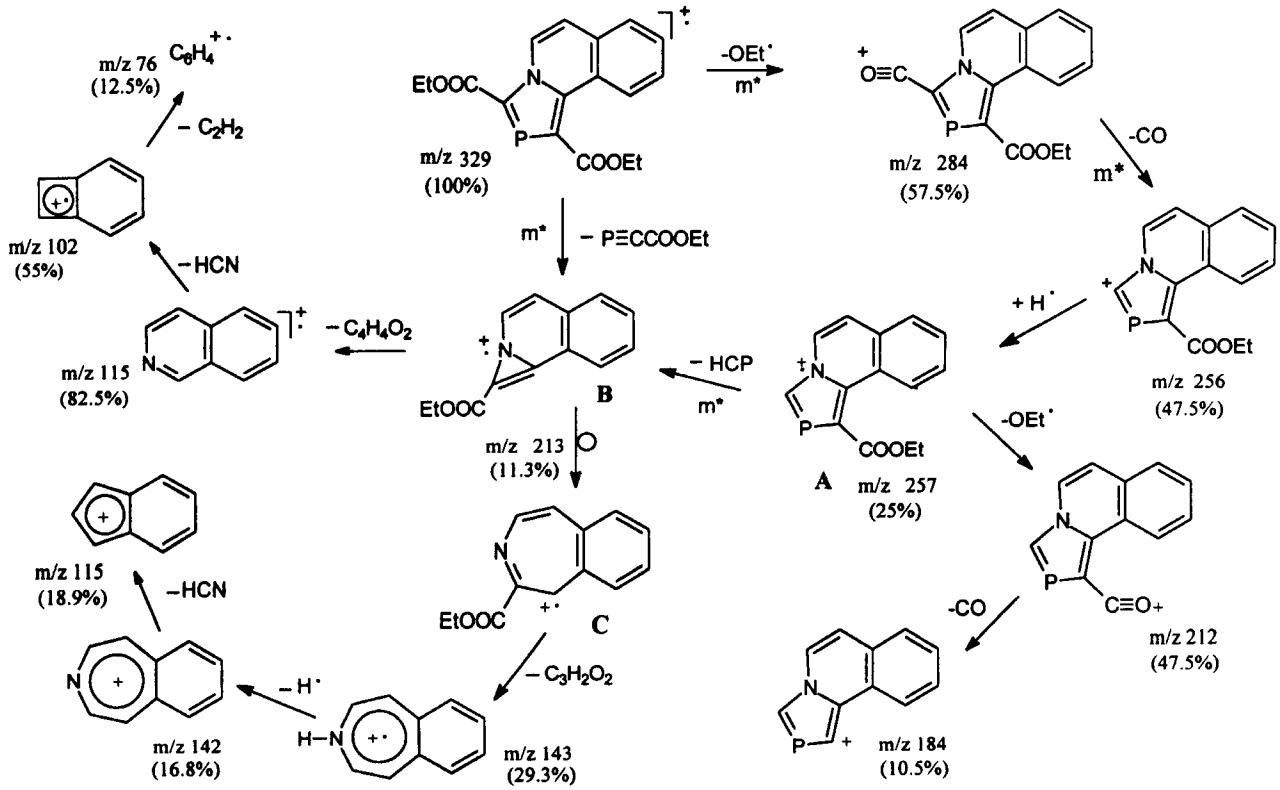
oxycarbonyl)[1,3]azaphospholo[5,1-*a*]isoquinoline **4b** reacts with 2,3-dimethyl-1,3-butadiene and sulfur in chloroform at ambient temperature to form the [2 + 4] cycloadduct **7** (Scheme 5).

The product **7** is a pale yellow solid, soluble in chloroform, methylene chloride, and acetonitrile. Its structure has been elucidated on the basis of ^{31}P, ^{1}H, and ^{13}C NMR data (Tables 1 and 2).

EXPERIMENTAL

All reactions involving phosphorus compounds were performed under a dry nitrogen atmosphere using the Schlenk technique. NMR spectra have been recorded on a JEOL EX 400 (^{31}P NMR at 161.8 MHz, ^{1}H NMR at 399.8 MHz, and ^{13}C NMR at 100.5 MHz) spectrometer or a Bruker ARX 300 (^{31}P NMR at 121.5 MHz, ^{1}H NMR at 300 MHz) spectrometer or a JEOL FX 90Q (^{31}P NMR at 36.23 MHz, ^{1}H NMR at 89.55 MHz) spectrometer. The chemical shifts refer to 85% H_3PO_4 (external) or tetramethylsilane (TMS) (internal). Mass spectra have been recorded on a Varian CH7 mass spectrometer, 70 eV at ambient temperature. Energy levels (eigenvalues) of frontier orbitals have been calculated by the semiempirical PM3 method using the MOPAC 6.0 package [21].

N-Alkylisoquinolinium bromides **1** were pre-



SCHEME 4 Mass spectral fragmentation of **4b.** The abundance of various ions as given in parentheses and the fragmentation steps that are supported by a metastable ion are marked m*.

pared by stirring isoquinoline with 1.1 equivalents of a suitably substituted methyl bromide in diethyl ether for 24–48 hours. The white to cream-colored solid thus obtained was filtered off, washed with dry diethyl ether (2 × 30 mL), and dried in vacuo.

1a: Yield 77%, m.p. 152–153°C; ^{1}H NMR ($CDCl_3$): δ = 3.71 (s, 3H, OCH_3), 6.43 (s, 2H, NCH_2), 7.66–8.48 (unresolved m, 5H, 4-H, 5-H, 6-H, 7-H, 8-H), 8.98 (d, 1H, $^3J_{HH}$ = 7.7 Hz, 3-H), 10.78 (s, 1H, 1-H).

1b: Yield 72%, m.p. 197–198°C, Lit m.p. 199°C [22]; ^{1}H-NMR ($CDCl_3$ + DMSO-d_6): δ = 1.30 (t, 3H, $^3J_{HH}$ = 7.1 Hz, CH_3), 4.27 (q, 2H, $^3J_{HH}$ = 7.1 Hz, OCH_2), 6.09 (s, 2H, NCH_2), 7.86–8.50 (unresolved m, 5H, 4-H, 5-H, 6-H, 7-H, 8-H), 8.84 (dd, 1H, $^3J_{HH}$ = 7.0 Hz, $^4J_{HH}$ = 1.4 Hz, 3-H), 10.61 (s, 1H, 1-H).

1c: Yield 60%, m.p. 207–208°C; ^{1}H-NMR ($CDCl_3$ + DMSO-d_6): δ = 6.76 (s, 2H, NCH_2), 7.51–8.49 (unresolved m, 10H, 4-H, 5-H, 6-H, 7-H, 8-H, *o*-H, *m*-H, *p*-H), 8.69 (d, 1H, $^3J_{HH}$ = 8.3 Hz, 3-H), 10.17 (s, 1H, 1-H).

1d: Yield 40%, m.p. 163–164°C; ^{1}H-NMR ($CDCl_3$ + DMSO-d_6): δ = 6.69 (s, 2H, NCH_2), 7.89–8.20 (unresolved m, 6H, 6-H, 7-H, *o*-H, *m*-H), 8.24 (d, 1H, $^3J_{HH}$ = 6 Hz, 4-H), 8.56 (d, 1H, $^3J_{HH}$ = 6.3 Hz, 5-H), 8.69 (d, 1H, $^3J_{HH}$ = 8.5 Hz, 8-H), 8.88 (d, 1H, $^3J_{HH}$ = 6.1 Hz, 3-H), 11.26 (s, 1H, 1-H).

1,3-Azaphospholo[5,1-a]isoquinoline **4:** *General Procedure*

To a well-stirred suspension of (0.05 mol) *N*-alkoxycarbonylisoquinolinium bromide **1** in 20 mL of toluene under an atmosphere of nitrogen at ambient temperature, 13.9 mL (0.10 mol) of $(C_2H_5)_3N$ was slowly added whereupon the reaction mixture turned cream-colored. After 10–20 minutes, a solution of 4.4 mL (0.05 mol) of PCl_3 in 10 mL of toluene was added dropwise over 45–60 minutes. The reaction mixture turned to light yellow, orange, and finally to red. After about 3 hours, an intense ^{31}P NMR signal at $\delta \sim 150$ indicated the formation of the *N*-isoquinolinium dichlorophosphinomethylide **2.** The reaction mixture was thereafter dried completely in vacuo, and the residue was extracted with diethyl ether (3 × 50 mL). All the ether extracts were combined, concentrated to about 15 mL, and kept in a refrigerator. A pale yellow solid that deposited was separated and dried. It gave a ^{31}PNMR signal at $\delta \sim$ 173–174 corresponding to 1,3-azaphospholo[5,1-*a*]isoquinolines, thus indicating the conversion of **2** into **4** during isolation.

To a suspension of *N*-alkylisoquinolinium bromide **1** (0.05 mol) in 40 mL of methylene chloride

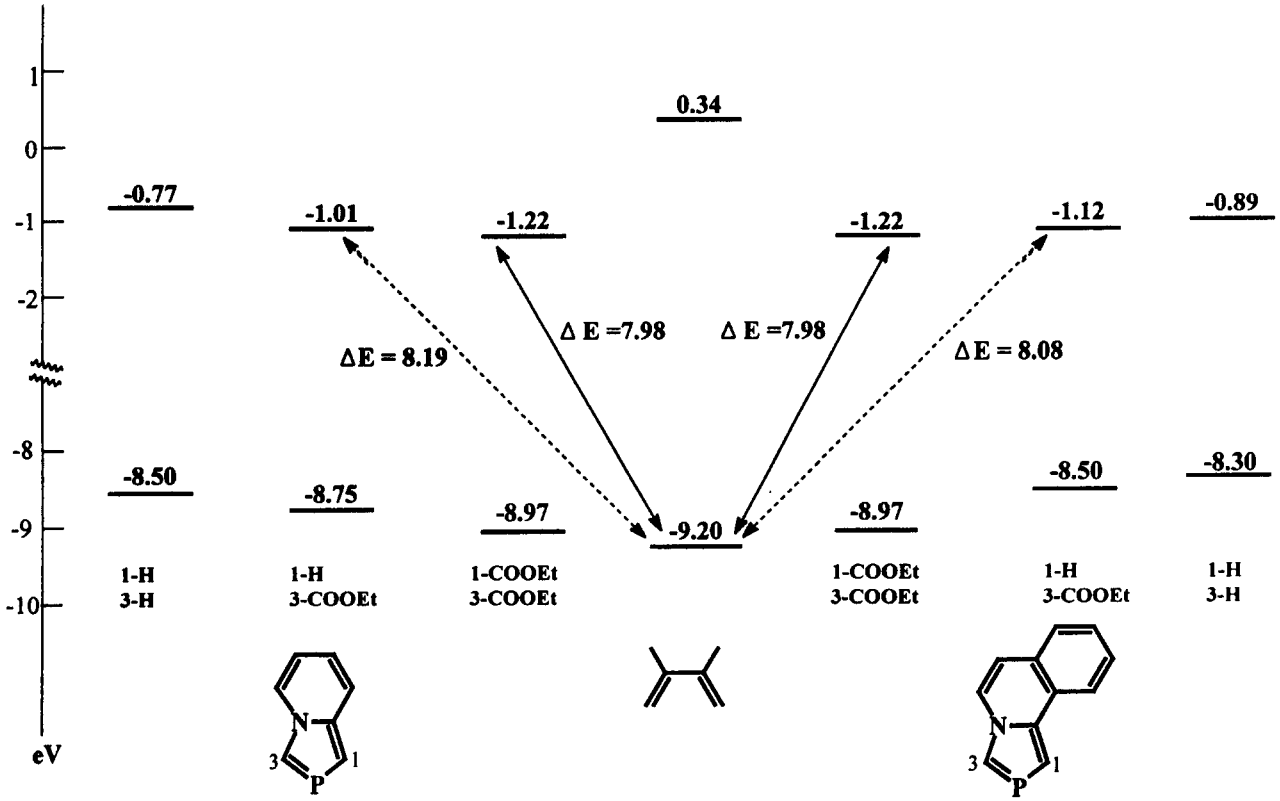
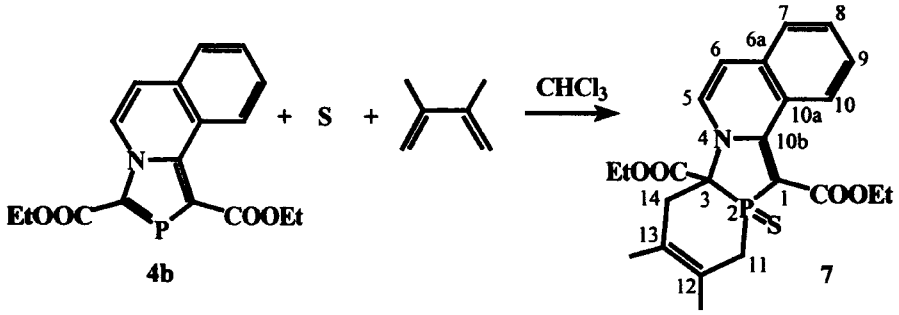


FIGURE 1 Frontier molecular orbitals of 2-phosphaindolizines, 2,3-dimethyl-1,3-butadiene, and 1,3-azaphospholo[5,1*a*]isoquinolines.



SCHEME 5

under dry nitrogen at ambient temperature, 13.9 mL (0.10 mol) of triethylamine was added with constant stirring. The color changed from cream to orange. After stirring for about 10–15 minutes, a solution of 2.2 mL (0.025 mol) PCl_3 in 15 mL CH_2Cl_2 was added dropwise. The stirring was continued for 4 hours, whereupon the color of the reaction mixture changed to dark brown. It was worked up according to the procedure previously described. **4b** was recrystallized from hot CH_3CN.

4a: Yield 28%, m.p. 96–97°C. Anal. calcd. for $C_{17}H_{16}NPO_4$ (329.2): C, 61.83; H, 4.88; N, 4.25. Found: C, 60.79; H, 4.77; N, 4.18.

4b: Yield 29%, m.p. 166–168°C.

Reaction of N-isoquinolinium Dichlorophosphino,methoxycarbonylmethylide **2a** *with N-(ethoxycarbonylmethyl)isoquinolinium Bromide* **1b**

N-Isoquinolinium dichlorophosphino, methoxycarbonylmethylide **2a** was generated in situ from the

reaction of 14.1 gm (0.05 mol) of *N*-(methoxycarbonylmethyl)isoquinolinium bromide **1b** with 13.9 mL (0.1 mol) of $(C_2H_5)_3N$ and 4.36 mL (0.05 mol) of PCl_3 in 50 mL of toluene at ambient temperature. To this mixture was added a suspension of 14.8 gm (0.05 mol) of *N*-(ethoxycarbonylmethyl)isoquinolinium bromide **1b** in 20 mL methylene chloride containing 13.9 mL (0.1 mol) triethylamine. The reaction mixture was stirred at ambient temperature overnight. The color of the reaction mixture changed from red to brown. The completion of the reaction was monitored by ^{31}P NMR spectroscopy. The reaction mixture was worked up as described previously.

Reaction of 1,3-Bis(ethoxycarbonyl)[1,3]azaphospholo[5,1-a]isoquinoline **4b** *with 2,3-Dimethyl-1,3-butadiene and Sulfur*

To a clear yellow solution of 1.64 gm (5 mmol) of **4b** in 25 mL of chloroform was added an excess amount of 2,3-dimethyl-1,3-butadiene (1.13 mL, 10 mmol) and 0.16 gm (5 mmol) of sulfur. After stirring at ambient temperature for 12 days, the ^{31}P-NMR spectrum of the reaction mixture indicated completion of the reaction and the formation of cycloadduct **7** with a ^{31}P NMR signal at $\delta = 69.5$. The yellow solid, obtained after evaporating the solvent and macerating the sticky mass so obtained with hexane, was recrystallized from hot CH_3CN.

7: Yield 90%, m.p. 130–135°C.

ACKNOWLEDGMENTS

Thanks are due to Dr. V. K. Jain for his helpful suggestions and to Dr. K. Karaghiosoff and Dr. M. K. Kindermann for providing some NMR spectra.

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