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REACTION OF VINYLPIRIDINES WITH OXAZOLES

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Depending on the structure, the reaction of the hydrochlorides of 2- and 4-vinylpyridines and 2-methyl-5-vinylpyridine with oxazoles leads to the synthesis of dipyridyls with or without a hydroxy group. It is shown that the regioselectivity of the reaction can be predicted on the basis of quantum-chemical calculations with the aid of the concepts of MO perturbation theory.

We have previously reported [1] that the reaction of oxazoles with 2- and 4-vinylpyridines (I and II) proceeds via the scheme of the Kondrat'eva reaction [2, 3] and leads to the production of dipyridyls. However, the relative orientation of the pyridine rings in the compounds obtained cannot be regarded as definitively established.

In the present research we made a theoretical estimate of the regioselectivity of the reaction of vinylpyridines with various oxazoles, realized this reaction, and determined the structures of the reaction products.

We have recently shown that the principal assumptions of MO perturbation theory [4] can be successfully used to predict the regioselectivity of processes involving cycloaddition to vinylpyridines [5]. Using the previously found quantum-chemical parameters of vinylpyridines [6] and our calculated† parameters of 2,4-dimethyloxazole (IIIa), 3,4-dimethyloxazole (IIIb), 2-methyl-4-phenyloxazole (IIIc), and β -(2-pyridyl)acrylic acid (IV) (Table 1) we estimated the perturbation energies of formation of regioisomeric adducts A and B with the aid of the known relationship [7]

$$\Delta E_{\pi} = 2 \left[\frac{(C_{Rn} \cdot C'_{Sm} \cdot \beta_{mn} + C_{Rp} \cdot C'_{Sq} \cdot \beta_{pq})^2}{|E_R - E'_S|} + \frac{(C'_{Rn} \cdot C_{Sm} \cdot \beta_{mn} + C'_{Rp} \cdot C_{Sq} \cdot \beta_{pq})^2}{|E'_R - E_S|} \right]$$

where C and C' are the coefficients of the atomic orbitals (AO) of the directly interacting n and p atoms (the diene, subscript R) and m and q atoms (the dienophile, subscript S) corresponding to the upper occupied molecular orbital (UOMO) and the lower vacant molecular orbital (LVMO), and E_R , E'_R and E_S , E'_S are the levels of the boundary orbitals of the diene (R) and the dienophile (S). An analysis of the values obtained (Table 2) showed that in the reaction of the hydrochlorides of vinylpyridines I and II and 2-methyl-5-vinylpyridine (V) with oxazoles IIIa-c the transition state that leads to the formation of regioisomer B is energetically more favorable. On the other hand, in the reaction of pyridylacrylic acid IV with oxazole IIIa one should expect the formation of regioisomer A. However, in the reaction of acid IV with oxazole IIIb the formation of both regioisomers A and B is virtually equally likely.

We accomplished the reaction of oxazoles IIIa-c, as well as 4-phenyloxazole (IIIId), 4-phenyl-5-methyloxazole (IIIe), 2-propyl-4-methyloxazole (IIIIf), 2,4,5-trimethyloxazole

*Deceased.

†The calculations were made by Yu. V. Gulevich with a BESM-6 computer by the MINDO/3 method.

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TABLE 1. Coefficients of the AO and Energies of the MO of Oxazoles IIIa-c and Acid IV

Compound	Boundary orbital	Coefficients of the AO of the C atoms			E, eV
		2	5	3	
IIIa	LVMO	-0,58412	-0,50271	—	1,8595
	UOMO	0,44670	-0,62198	—	-8,1488
IIIb	LVMO	0,48598	-0,56465	—	1,7872
	UOMO	0,44657	-0,59942	—	-8,1151
IIIc	LVMO	0,06958	0,41221	—	0,9802
	UOMO	-0,33425	0,56387	—	-9,1870
IV*	LVMO	-0,46073	0,49952	-0,24411	-0,0415
	UOMO	0,44591	0,25656	-0,40306	-9,0038

*In the case of acid IV atoms 2 and 5 correspond to the β and α atoms of the side chain. Atom 3 corresponds to the C_3 atom of the pyridine ring.

TABLE 2. Energies of Formation (ΔE_{π}) of Regioisomers A and B* (kJ/mole)

Hetero-diene	Dienophile							
	I		II		IV		V	
	A	B	A	B	A	B	A	B
IIIa	62,2	71,8	80,9	93,1	111,0	106,4	56,4	58,3
IIIb	20,1	29,4	20,3	31,2	75,7	76,4	1,7	3,1
IIIc	17,8	25,5	21,6	32,1	53,4	56,6	11,6	13,5

*The quantum-chemical parameters for the protonated forms of I, II, and V and the neutral form of IV were used in the calculation.

(IIIg), 4-methyl-5-ethoxyoxazole (IIIh), 2-phenyl-5-ethoxyoxazole (IIIi), and 5-methyl-4-hexyloxazole (IIIj) with vinylpyridines I, II, and V, as well as with acid IV, by refluxing a solution of a twofold excess of the dienophile with the corresponding oxazole in n-butyl or isoamyl alcohol. The use of other solvents such as water, ethylene glycol, ethanol, dioxane, or dimethylformamide (DMF) leads only to lowering of the yields of the final products.

An analysis of the resulting compounds showed that 3-hydroxy-5-pyridylpyridines (VIa-g) are formed in the reaction of vinylpyridines I, II, and V with 5-unsubstituted oxazoles (ex-

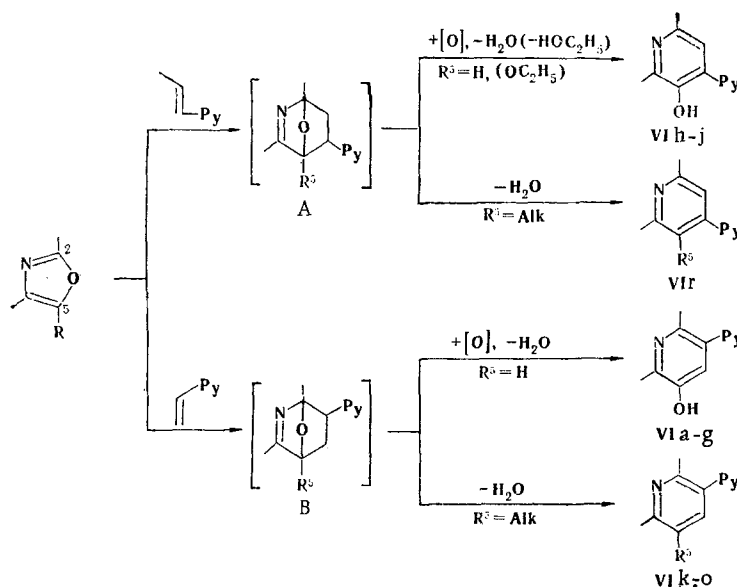
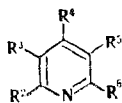


TABLE 3. Properties of Dipyriddyis VIa-q



Com- pound	R ²	R ³	R ⁴	R ⁵	R ⁶	mp, °C	UV spec- trum, ^a λ _{max} , nm (log ε)	Found, %		Empirical formula	Calc., %		Yield, %
								C	H		C	H	
VIa	CH ₃	OH	H	Py-2b	CH ₃	242—244	297 (4,2)	72,3	6,1	C ₁₂ H ₁₂ N ₂ O	72,0	6,0	60
VIb	CH ₃	OH	H	Py-2	C ₃ H ₇	130—132	297 (4,3)	73,2	7,1	C ₁₄ H ₁₆ N ₂ O	73,6	7,0	12
Vic	C ₆ H ₅	OH	H	Py-2	H	220—222	240 (4,4), 320 (4,3)	77,0	4,9	C ₁₆ H ₁₂ N ₂ O	77,4	4,9	50
VIc	C ₆ H ₅	OH	H	Py-2	CH ₃	202—204	242 (4,4), 324 (4,4)	77,6	5,3	C ₁₇ H ₁₄ N ₂ O	77,8	5,4	66
VIe	C ₆ H ₅	OH	H	Py-4	H	255—256	245 (4,1), 321 (3,9)	77,8	5,1	C ₁₆ H ₁₂ N ₂ O	77,4	4,9	42
VIe	C ₆ H ₅	OH	H	Py-4	CH ₃	267—269	239 (4,0), 318 (4,3)	78,1	5,4	C ₁₇ H ₁₄ N ₂ O	77,8	5,4	25
VIg	C ₆ H ₅	OH	H	Py-3	CH ₃	230—232	240 (4,3), 311 (4,3)	78,1	5,8	C ₁₈ H ₁₆ N ₂ O	78,2	5,8	20
VIh	CH ₃	OH	Py-2	H	H	86—87	252 (4,0), 285 (3,9), 325 (3,8)	71,0	5,7	C ₁₁ H ₁₀ N ₂ O	70,9	5,4	45
VIi	H	OH	Py-2	H	C ₆ H ₅	126—127	—	77,2	4,8	C ₁₆ H ₁₂ N ₂ O	77,4	4,9	2, f
VIj	CH ₃	OH	Py-2	H	CH ₃	83—84	256 (4,1), 282 (3,9), 336 (3,8)	71,6	5,7	C ₁₂ H ₁₂ N ₂ O	72,0	6,0	12
VIk	CH ₃	CH ₃	H	Py-2	H	185—186	262 (3,8), 268 (3,7)	52,0	3,9	C ₁₈ H ₁₅ N ₅ O ₇	52,3	3,7	25
VIl	CH ₃	CH ₃	H	Py-2	CH ₃	76—77	262 (3,9), 268 (4,0)	78,6	7,2	C ₁₃ H ₁₄ N ₂	78,8	7,1	25
VI m	C ₆ H ₅	CH ₃	H	Py-2	H	77—78	262 (3,9), 267 (3,9)	82,8	5,6	C ₁₇ H ₁₄ N ₂	83,0	5,6	80
VI n	CH ₃	C ₆ H ₁₃	H	Py-2	H	146—147	262 (3,9), 266 (3,8)	56,8	5,3	C ₂₃ H ₂₅ N ₅ O ₇	57,1	5,2	37
VI o	C ₆ H ₅	CH ₃	H	Py-3	H	108—109	263 (3,9), 270 (4,0)	82,9	6,0	C ₁₈ H ₁₆ N ₂	83,0	6,2	3
VI p	C ₆ H ₅	OCH ₃	H	Py-2	CH ₃	128—129	230 (4,9), 290 (4,5)	78,3	5,7	C ₁₈ H ₁₆ N ₂ O	78,2	5,8	19
VI q	C ₆ H ₅	OTos ^e	H	Py-2	CH ₃	108—109	230 (4,9), 292 (4,6)	69,2	4,9	C ₂₄ H ₂₀ N ₂ O ₃ S	69,2	4,8	60

^aIn methanol. ^b2-Pyridyl is indicated by Py-2, Py-4 is 4-pyridyl, and Py-3 is 6-methyl-3-pyridyl. ^cThe picrate. The base had bp 168–170°C (12 mm). ^dThe picrate. The base had bp 161–163°C (9 mm). ^eThe tosylate, which was obtained from 2 mmole of VI d and 5 mmole of p-toluenesulfonyl chloride in 10 ml of 20% sodium hydroxide solution.

cept for oxazoles IIIh and IIIi), whereas in the reaction of the same vinylpyridines with 5-substituted oxazoles (except for IIIh and IIIi) the reaction products (VIk-o) do not contain a hydroxy group (see Table 3 for the properties of VI).

Hydroxydipyriddyis VIc-g have similar UV spectra with two maxima at 240 and 320 nm. The long-wave maximum in the UV spectra of these compounds in solution in alcohol alkali undergoes a 36-nm bathochromic shift.

Moreover, methylation or tosylation of the hydroxy group in VI d (to give VI p and VI q) leads to a 20-nm hypsochromic shift of the long-wave band. These spectral properties are very characteristic for 2-phenyl-3-hydroxypyridines [8].

It follows unambiguously from an analysis of the PMR spectra (Table 4) that the pyridine residue in them is located in position 5 of the hydroxypyridine ring [doublets of 2-H protons at 8.88 and 8.63 ppm, as well as 4-H protons at 8.63 and 7.70 ppm, respectively, for IVc and IVe, with identical spin-spin coupling constants (SSCC) of 2 Hz]. Since the UV spectra of VIa-f are similar to one another, all of them are apparently 3-hydroxy-5-pyridylpyridines.* At the same time, VIh, which was obtained by reaction of vinylpyridine I with

*The long-wave band in the UV spectra of VIa, b is shifted hypsochromically 23 nm as compared with the corresponding band in the spectrum of VIe; this is analogous to a comparison of the UV spectra of 2-phenyl-3-hydroxypyridine and 3-hydroxypyridine [8].

TABLE 4. PMR Spectra and Mass Spectra of VIa-f, h, j-m

Com- pound	PMR spectrum: * group, δ (ppm), multiplicity [No. of protons, spin-spin coupling constant (Hz)]						Mass spectrum, † m/e (relative intensity, %)
	R ^c	R ³	R ⁴	R ⁵	R ⁶		
VIa	CH ₃ , 2.05 s	OH, 3.20 s	H, 7.20 s	Py-2, 8.55 q (1H; 2.0; 5.0); 7.78 q (1H; 2.0; 8.0), 7.48 d (1H, 8.0), 7.35 q (1H, 5.0; 8.0)	CH ₃ , 2.47 s	200 (100), 199 (19), 185 (9), 171 (30), 158 (10), 131 (26), 130 (66), 91 (16), 79 (19), 78 (32), 77 (36)	
VIb	CH ₃ , 2.10 s	OH, 3.25 s	H, 7.15 s	Py-2, 8.58 q (1H; 2.0; 5.0); 7.80 q (1H; 2.0; 8.0), 7.50 d (1H, 8.0), 7.40 q (1H, 5.0; 8.0)	-CH ₂₋ , 3.50 t	228 (38), 227 (35), 213 (53), 211 (9), 200 (84), 199 (100), 198 (42), 169 (9), 130 (9), 107 (18), 78 (19)	
VIc	C ₆ H ₅ , 8.12 d (2H), 7.40 m (3H)	OH, 3.50 s	H, 8.07 d (1H; 2.0)	Py-2, 8.70 q (1H; 2.0; 5.0); 8.02 d (1H, 8.0), 7.92 t (1H; 2.0; 8.0), 7.40 q (1H; 8.0; 5.0)	H, 8.88 d (1H, 2.0)	248 (84), 247 (100), 220 (32), 219 (23), 193 (8), 192 (13), 191 (9), 117 (18), 116 (10), 115 (10), 78 (23)	
VI d	C ₆ H ₅ , 8.10 d (2H), 7.45 m (3H)	OH, 3.30 s	H, 7.22 s	Py-2, 8.68 q (1H; 2.0; 5.0); 7.88 q (1H; 2.0; 8.0), 7.50 d (1H, 8.0), 7.37 q (1H, 5.0; 8.0)	CH ₃ , 2.40 s	262 (78), 261 (100), 234 (10), 233 (16), 150 (11), 132 (9), 130 (22), 104 (103), 103 (7), 78 (12), 77 (11)	
VIe	C ₆ H ₅ , 8.07 d (2H), 7.45 m (3H)	OH, 3.30 s	H, 7.62 d (1H; 2.0)	Py-4, 8.68 d (2H; 5.0), 7.70 d (2H; 5.0)	H, 8.57 d (1H, 2.0)	248 (88), 247 (100), 246 (9), 220 (21), 219 (8), 117 (8), 116 (10), 104 (18), 103 (28), 90 (11), 78 (9)	
VI f	C ₆ H ₅ , 8.10 d (2H), 7.30 m (3H)	OH, 3.30 s	H, 7.15 d	Py-4, 8.70 d (2H, 5.0), 7.75 d (2H, 5.0)	CH ₃ , 2.36 s	262 (100), 261 (91), 260 (9), 234 (35), 233 (38), 232 (8), 158 (6), 131 (9), 130 (11), 103 (7), 78 (14)	

VIh	CH ₃ , 2.44 s	OH, 3.30 s	Py-2, 8.87 q (1H: 2.0; 5.0), 8.34 d (1H, 8.0), 8.0 sext, (1H, 8.0, 2.0), 7.67 m (1H)	H, 7.78 td (1H: 5.0)	H, 8.01 d (1H: 5.0)	186 (100), 185 (15), 158 (16), 157 (51), 145 (13), 130 (15), 117 (48), 104 (10), 90 (19), 89 (26), 78 (20)
VIj	CH ₃ , 2.25 s	OH, 3.40 s	Py-2, 8.90 q (1H, 2.0; 5.0), 8.16 d (1H, 8.0), 7.55 sext (8.0; 2.0), 7.45 m (1H)	H, 7.40 s	CH ₃ , 2.40 s	200 (100), 199 (16), 185 (4), 172 (6), 171 (16), 159 (8), 130 (30), 129 (31), 119 (5), 103 (6), 78 (5)
VIk	CH ₃ , 2.60 s	CH ₃ , 2.35 s	H, 8.50 d (1H: 2.0)	Py-2, 9.10 q (1H, 2.0; 5.0), 8.20 m (1H), 7.50 m (2H)	H, 9.30 d (1H, 2.0)	184 (75), 183 (100), 182 (14), 169 (18), 108 (9), 142 (25), 141 (15), 140 (10), 117 (24), 115 (10), 104 (8)
VIl	CH ₃ , 2.42 s	CH ₃ , 2.11 s	H, 7.2 s	Py-2, 8.90 d (1H, 5.0), 7.4-7.6 m (3H)	CH ₃ , 2.46 s	198 (60), 197 (100), 196 (25), 183 (20), 182 (10), 156 (14), 155 (12), 142 (10), 129 (10), 128 (12), 78 (10)
VI m	C ₆ H ₅ , 7.6-7.8 m (5H)	CH ₃ , 2.1 s	H, 8.02 d (1H: 2.0)	Py-2, 8.88 q (1H, 2.0; 5.0), 7.35 m (1H), 7.6-7.8 m (2H)	H, 8.73 d (1H: 2.0)	246 (52), 245 (100), 244 (17), 243 (10), 219 (5), 218 (7), 217 (12), 165 (9), 142 (7), 141 (6), 80 (11)

*In deuterodimethyl sulfoxide with hexamethyldisiloxane as the standard.

†The molecular-ion peak and the 10 most intense peaks are presented.

oxazole IIIh, has a UV spectrum that differs markedly from the spectrum of VIa. In it one observes three absorption bands at 252, 285, and 325 nm, which is similar to what is observed for aryloxy pyridines, which exist partially in the form of dipolar ions [8]. This makes it possible to assume that the hetaryl residue in VIh is adjacent to the hydroxy group, i.e., in the 4 position. In fact, two doublets of 2-H (8.01 ppm) and 3-H (7.78 ppm) protons with an identical SSCC of 5.0 Hz are observed in the PMR spectrum of VIh in the weak-field region. The shift of the 2-H signal to stronger field as compared with the pyridine derivatives is apparently associated with the presence of a hydroxy group in the para position relative to it, while the shift of the 3-H signal to weaker field is explained by the effect of an adjacent electron-acceptor pyridine ring. The reaction of oxazole IIIa with acid IV gave VIj, which does not contain a carboxy group and is similar to VI with respect to the results of analysis and its mass spectrum but differs with respect to its melting point and UV spectrum. At the same time, its UV spectrum was similar to the UV spectrum of hydroxydipyridyl VIh. In addition to the characteristic pattern of signals of a 2-pyridyl residue, a singlet of a 5-H proton at 7.40 ppm was observed in the PMR spectrum of the substance obtained. The weak-field shift of β -H as compared with α -picoline in this case is associated with the presence of an adjacent hetaryl residue. The mass-spectral behavior of dipyridyls VIa and VIj is very similar, since primary fragmentation of their molecular ions commences with the loss of a CHO fragment and the formation of identical ions with m/e 171 in both cases. Thus, in complete agreement with the calculations (Table 2), regioisomers of the B type are formed in the reaction of vinylpyridines I, II, and V with 5-unsubstituted oxazoles. At the same time, in agreement with the data in Table 2, a regioisomer of the A type is formed in the reaction of acid IV with oxazole IIIa. As regards 5-alkoxyoxazoles IIIh and IIIi, it is known from the literature [3, 9] that 4-substituted 3-hydroxypyridines are always formed in the reaction with unsymmetrical dienophiles of the acrylic acid derivative type; this is also in good agreement with the calculated data [10]. In the light of the material set forth above, the dipyridyls and hydroxydipyridyls that we previously obtained [11] in the reaction of 2-methyl-4-tert-butyloxazole with 2-vinylpyridine should also be classified as 3-hydroxy-5-pyridylpyridines, since their UV spectra also (like that of VIa) contain only one absorption band at 297 nm.

The reaction of 5-alkyl-substituted oxazoles IIIb, e, g, j with vinylpyridines I, II, and V led to the formation of dipyridyls VIj-o, which do not contain a hydroxy group. Two close-lying absorption maxima at 262 and 268-270 nm, which are characteristic for derivatives of dipyridyls [11], are observed in their UV spectra. An analysis of the PMR spectra of dipyridyls VIk-m (Table 4) makes it possible to assert that they have the 2,3-dipyridyl structure; this is also in good agreement with the data in Table 2.

A substance that does not contain a carboxy group and, according to analysis, corresponds to dipyridyl VIk was isolated in 7% yield in the form of an oil in the reaction of acid IV with oxazole IIIb; however, the picrate of this compound has a lower melting point, and chromatographic mass-spectral analysis of the oil shows the presence of a mixture of two substances in a ratio of 3:2. Both compounds have a molecular mass of 184 and are extremely similar with respect to the character of the fragmentation of their molecular ions. According to its retention time and mass spectrum, the second compound corresponds to VIk. Signals of protons of both VIk and the isomeric 2,3-dimethyl-4-(2-pyridyl)pyridine (VIr) are observed at strong field in the PMR spectrum of the mixture obtained.

These data make it possible to conclude that the regiospecificity of the reaction of both 5-substituted and 5-unsubstituted oxazoles with acid IV is also in conformity with the theoretical predictions (Table 2), while decarboxylation takes place in the second step of the process after the formation of the primary adduct.

Thus the use of the computational methods of MO perturbation theory makes it possible to successfully predict the regiospecificity of the Kondrat'eva reaction.

EXPERIMENTAL

The UV spectra of methanol solutions of the compounds were recorded with a Cary-15 spectrophotometer. The PMR spectra were obtained with Varian T-60 and Bruker WP-200 and WP-360 spectrometers. The mass spectra were recorded with MKh-1303 and Varian MAT-111 spectrometers at energies of 50 and 80 eV, respectively, with direct introduction of the substances into the ion source. The chromatographic mass spectra were obtained with an MAT-111 spec-

trometer with a 1.5-m long column filled with 3% SE-30 on Chromosorb with programmed heating from 100 to 250°C at a rate of 10 deg/min.

We have previously described [13] the synthesis of oxazoles IIIc-g, j. Oxazole IIIh was obtained by the method in [14], while oxazole IIIi was obtained by the method in [15]. Acid IV was synthesized by condensation of 2-formylpyridine with malonic acid [16]. According to the results of gas-liquid chromatography (GLC), vinylpyridines I, II, and V were more than 98% pure. Their hydrochlorides were obtained by passing dry hydrochloric acid through a solution of the corresponding vinylpyridine in absolute ether. The melting points of the hydrochlorides were as follows: 119-120°C for I, 223-225°C for II, and 164-165°C for V. According to the data from the PMR spectrum, acid IV has a trans configuration.

Reaction of Vinylpyridines with Oxazoles III. A solution of 25 mmole of the oxazole and 55 mmole of vinylpyridine hydrochloride in 30 ml of n-butyl or isoamyl alcohol was refluxed for 5-8 h, after which it was allowed to stand overnight. The solvent was evaporated, and the residue was dissolved in water. The unchanged oxazole III was extracted with ether, and the aqueous layer was neutralized with 2 N sodium hydroxide solution to pH 7-7.5. Dipyriddyds VIa-g, l, m, o precipitated from the reaction mixtures and were separated and recrystallized. Dipyriddyds VIk, n were extracted with ether, the extract was dried with anhydrous magnesium sulfate, the solvent was evaporated, and the residue was distilled in vacuo. The properties of VI are presented in Table 3. The reaction of the hydrochloride of I with oxazoles IIIh and IIIi, as well as the reaction of acid IV with oxazoles IIIa and IIIc, was carried out in acetic acid for 8 h (or, respectively, 25 h), and the mixture obtained after evaporation of the solvent and neutralization with sodium carbonate was extracted with hot hexane (VIh and VIj) or chloroform (VIi).

3-Methoxy-2-phenyl-6-methyl-5-(2-pyridyl)pyridine. A 1.3-g (5 mmole) sample of dipyriddydl VIId and 1.4 g (10 mmole) of methyl iodide were added at 20°C to a solution of 0.2 g of sodium metal in 10 ml of absolute ethanol. After 2 days, the alcohol was removed by distillation, a 1 N solution of sodium hydroxide was added to pH 9-10, and VIP was separated. See Table 3 for the yields and properties.

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