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CYCLODIMERIZATION OF VINYLPYRIDINES

P. B. Terent'ev, V. G. Kartsev,
A. V. Gorelov, I. P. Gloriozov,
Yu. A. Gulevich, and A. N. Kost*

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When isomeric 2- and 4-vinylpyridines, as well as 2-methyl-5-vinylpyridine, are heated in polyphosphoric or acetic acid, they undergo dimerization, which proceeds via a 1,4-cycloaddition scheme to give pyridyl-substituted 5,6,7,8-tetrahydroquinolines or isoquinolines. Quantum-chemical calculations with the use of the concepts of molecular orbital perturbation theory make it possible to predict the regiospecificity of the reaction. The regiospecific cross cycloaddition of 4-vinylpyridine to 2-methyl-5-vinylpyridine was proposed theoretically and proven experimentally.

In 1967 Winterfeld and Nann [1], in the course of dehydration of 2-(2-hydroxyethyl)-pyridine in polyphosphoric acid (PPA) unexpectedly obtained 5-(2-pyridyl)-5,6,7,8-tetrahydroquinoline, the formation of which they explained by dimerization of the initially formed 2-vinylpyridine via the scheme of the diene synthesis. However, no proof for this assumption was presented in [1]. In addition, the boundaries of applicability of this reaction and the problems of its regioselectivity remained unclear.

We studied the processes involved in the cyclodimerization of substituted 2-vinylpyridines (Ia-f), as well as 2-methyl-5-vinyl- and 4-vinylpyridines (II and III, respectively). We found that the reaction is quite selective with respect to the selection of the solvent and proceeds successfully only in acids of medium strength such as acetic, polyphosphoric, etc. Dimerization is not observed in strong acids (sulfuric and hydrochloric) or in neutral and basic solvents [nitrobenzene, hexametapol, and dimethylformamide (DMF)]. This makes it possible to assume that the protonated vinylpyridine molecule acts as the dienophile in the dimerization reaction, while the unprotonated vinylpyridine molecule acts as the diene. An increase in the "dienophile" activity of 2- and 4-vinylpyridines when they are protonated has already been noted [2]. This also explains the success of the reaction on passing from DMF to polyphosphoric acid (PPA). Strong electrostatic repulsion of each pair of such molecules occurs in strongly acidic media, in which all of the vinylpyridine molecules are protonated, and this constitutes a hindrance to dimerization.

Considering the fact that the molecules of vinylpyridines I contain two pseudodiene systems, viz., N=C—C=O and C=C—C=C, one must assume that the formation of four regiospecific compounds is fundamentally possible during their dimerization (Table 2).

In recent years the regioselectivity of electrocyclic reactions and, in particular, the reactions of the diene synthesis has been predicted successfully by means of the computational methods of molecular orbital (MO) perturbation theory [3]. We recently demonstrated

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*Deceased.

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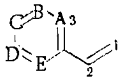
TABLE 1. Coefficients of the Atomic Orbital and Energy Levels of the Upper Occupied Molecular Orbitals (UOMO) and Lower Vacant Molecular Orbitals (LVMO) of Vinylpyridines Ia, III, and IV



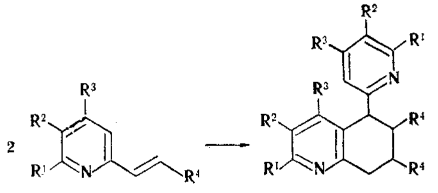
Vinyl-pyridines*	Form†	Boundary orbitals	Coefficients of the AO of the C atoms			E, eV
			1	2	3	
Ia, E =N	N	LVMO	−0,453	0,312	−0,149	0,707
		UOMO	−0,436	−0,306	0,401	−8,605
	P	LVMO	0,277	−0,067	0,080	−4,957
		UOMO	−0,498	−0,466	0,403	−13,623
Ia, A=N	N	LVMO	0,449	−0,302	0,411	0,726
		UOMO	0,436	0,312	−0,202	−8,587
	P	LVMO	0,281	−0,075	0,483	−4,989
		UOMO	0,498	0,453	−0,158	−13,670
IV, D=N	N	LVMO	−0,402	0,279	−0,460	0,770
		UOMO	0,472	0,331	−0,221	−8,550
	P	LVMO	0,083	−0,016	0,554	−4,995
		UOMO	−0,564	−0,527	0,241	−13,362
IV, B =N	N	LVMO	−0,402	0,281	−0,109	0,763
		UOMO	0,472	0,329	−0,362	−8,553
	P	LVMO	−0,081	0,017	−0,434	−5,005
		UOMO	−0,566	−0,522	0,355	−13,381
III, C=N	N	LVMO	0,432	−0,283	0,280	0,611
		UOMO	0,490	0,368	−0,326	−8,787
	P	LVMO	0,300	−0,047	0,136	−5,026
		UOMO	−0,584	−0,576	0,304	−13,618

*The letters =CH are not indicated.
†Abbreviations: N is neutral, and P is protonated.

the possibility of their use as applied to cycloaddition reactions on the basis of vinylpyridines [4].

Using the MINDO/3 quantum-chemical method,* we calculated the coefficients of the atomic orbitals (AO) and the energy levels of the upper occupied and lower vacant molecular orbitals (UOMO and LVMO, respectively) of the neutral and protonated forms of I, III, and 3-vinylpyridine (IV) (Table 1). The energies of the π-electron stabilization (ΔE_π) of the regioisomers, the formation of which is theoretically possible in the case of dimerization of various vinylpyridines, were calculated from these data by means of the well-known formula [6]. It follows from an analysis of the data in Table 2 that the formation of only one of the regioisomers (Va and VI, respectively) is most probable in the dimerization of vinylpyridines Ia and III.

Having accomplished the dimerization of Ia-f and III by heating in PPA at 180-200°C for 2 h, we found after chromatographic mass-spectral analysis of the reaction mixtures obtained that only one compound is formed in all cases. Their mass-spectral fragmentation corresponds to the proposed Va-f and VI structures (Table 3):



Ia-f V a-f

The PMR spectra of Va-e are very similar. A triplet of one 5-H proton at 4.46-4.53 ppm, a triplet of two 8-H protons at 3.24-3.27 ppm, and a multiplet of four 6-H and 7-H protons

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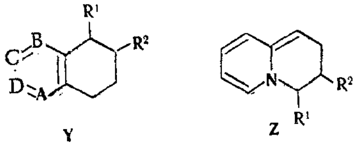
*The calculation was made with a BÉSM-6 computer with the aid of a TOPEAMOP program [5].

TABLE 2. ΔE_π Values for the Possible Products of Cyclodimerization of Vinylpyridines Ia, III, and IV and Products of the Cross Reaction of III and IV



Y Z

Reacting vinyl-pyridines	Adduct*				ΔE_π, kJ /mole
	compound	form	R¹	R²	
Ia+Ia	Va, A=N	Y	Py-2†	H	41,4
	A=N	Y	H	Py-2	36,1
		Z	Py-2	H	32,8
		Z	H	Py-2	24,4
IV+IV	VIIIa, D=N	Y	Py-3	H	14,8
	VIIIb, D=N	Y	H	Py-3	13,3
	VIIa, B =N	Y	Py-3	H	37,8
	VIIb B =N	Y	H	Py-3	38,3
III+III	VI, C=N	Y	Py-4	H	45,0
	C=N	Y	H	Py-4	37,4
III+IV	IXa, D =N	Y	Py-4	H	33,2
	IXb, D=N	Y	H	Py-4	25,8
	Xa, B =N	Y	Py-4	H	56,6
	Xb, B =N	Y	H	Py-4	46,0
	XIa, C =N	Y	Py-3	H	27,0
	XIb, C =N	Y	H	Py-3	25,6

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*The letters =CH are not indicated.

†Pyridyl is indicated by Py.

TABLE 3. 5-(2-Pyridyl)-5,6,7,8-tetrahydroquinolines (Va-e)

Compound	R² *	mp, °C	R_f†	Mass spectra of the bases, m/e (intensity in percent relative to the maximum peak)‡	Found, %		Empirical formula	Calc., %		Yield, %
					C	H		C	H	
Va	H	44—46	0,30	210 (92), 209 (39), 195 (18), 182 (18), 181 (100), 132 (24), 131 (21), 130 (39), 118 (32), 117 (32), 93 (32)	79,9	6,6	$C_{14}H_{14}N_2$	80,0	6,7	36
Vb	H	189—190**	0,45	238 (70), 237 (28), 223 (13), 210 (13), 209 (18), 146 (18), 144 (17), 132 (100), 107 (22), 102 (17), 94 (30)	80,7	7,5	$C_{16}H_{18}N_2$	80,7	7,6	43
Vc	CH_3	191—193**	0,32	238 (100), 237 (40), 223 (20), 210 (20), 209 (79), 146 (21), 145 (26), 144 (32), 132 (22), 118 (16), 107 (28), 94 (35)	80,6	7,5	$C_{16}H_{18}N_2$	80,7	7,6	40
Vd	C_2H_5	178—180**	0,41	266 (100), 265 (28), 238 (29), 237 (87), 160 (22), 159 (24), 158 (32), 146 (27), 129 (45), 121 (32), 108 (40)	81,0	8,7	$C_{18}H_{22}N_2$	81,2	8,6	42
Ve	H	180—182**	0,36	238 (100), 237 (32), 223 (16), 210 (16), 209 (27), 146 (19), 144 (20), 129 (75), 107 (24), 94 (32)	80,6	7,5	$C_{16}H_{18}N_2$	80,7	7,6	30

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*For Va, c-f, R^1 = H; for Vb, R^1 = CH_3; for Va-d, f, R_3 = H; for Ve, R^3 = CH_3; for If and Vf, R^4 = CH_3; for Va-e, R^4 = H.

†In a benzene—methanol system (9:1).

‡The peaks of the ions of the bases with intensities ≥ 10% are presented.

**Methiodide.

at 2.1-2.5 ppm are observed in them. The molecular ions of Va-e eliminate a hydrogen atom or a residue of the corresponding pyridine. In addition, the retrodiene fragmentation of the molecular ions leads to [M—28] ions with the elimination of C_6 and C_7 atoms, and this confirms the structure of Va-e.

In conformity with this, the peak of an ion with mass 182* ([M—C_4H_8]) is observed in the mass spectrum of Vf, and this proves the presence of two methyl groups in the 6 and 7 positions.

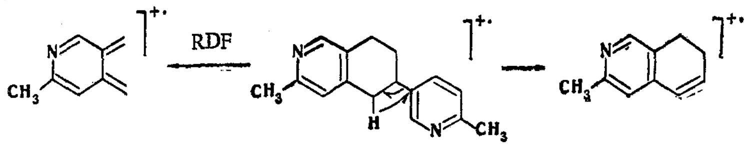
The PMR spectrum of VI contains a triplet of one 8-H proton at 4.27 ppm, a broad triplet of two 5-H protons at 3.1 ppm, and a multiplet of four 6-H and 7-H protons at 2.0-2.3 ppm; these data correspond only to structure VI. The presence of an [M—28] ion peak in the mass spectrum confirms its structure.

An analysis of the data in Table 2 also makes it possible to assume that in the dimerization of vinylpyridine II (IV) one should expect preferred cyclization with the participation of the 4 position of the pyridine ring (VII). At the same time, the ΔE_π values of regioisomers VIIa and VIIb are close. Proceeding from this, in the dimerization of vinylpyridine II one should expect the principal formation of a mixture of these compounds.

A chromatographic mass-spectral study of the reaction mixture obtained after heating vinylpyridine II in PPA, alkalization, and extraction with chloroform demonstrated the presence of three compounds, viz., VIIIa, VIIb, and VIIa, in the extract in a ratio of 3:5:2.

The same ion peaks (M = 238) are observed in the mass spectra of all three compounds; however, differences are noted in the subsequent fragmentation of these ions (Table 4). Thus the presence of intense peaks of [M—H] and [M—C_2H_5] ions is characteristic for the fragmentation of VIIIa. It is known that the most intense peaks of [M—H] ions are characteristic for 2-ethyl- [7] or 2-phenyl- [8] and 2-benzylpyridines [9], and this confirms the correctness of the assigned structure. This conclusion is also in agreement with the shortest chromatographic retention time for VIIIa.

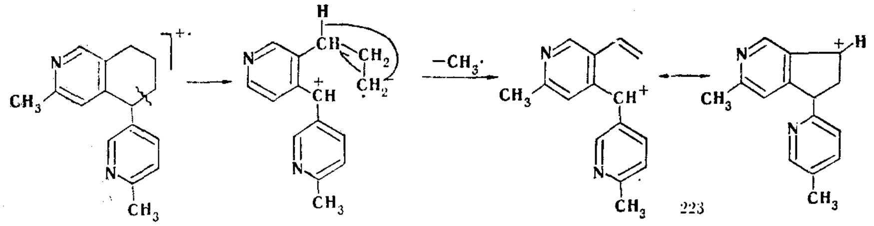
Especially effective elimination of a molecule of methylpyridine, which takes place with the transfer of one hydrogen atom (the [M—93] ion with mass 145) and, simultaneously, the relatively high intensity of the [M—119] ion peak (retrodiene fragmentation) are characteristic for the dissociative ionization of VIIb.



119 VIIb 145

RDF — retrodiene fragmentation

Finally, VIIa readily eliminated a methyl group under the influence of electron impact, and this is in good agreement with the proposed structure, since in this case the positive charge in any of the structures of the F_1 and F'_1 ions is found adjacent to the electron-enriched β-position of the pyridine ring:



VIIa F_1 F'_1

In conformity with this, two singlets of methyl groups at 2.76 and 2.83 ppm with an area ratio of ∿2:1, two triplets of 5-H (VIIa) and 8-H (VIIIa) methylidyne protons at 4.11 and 3.86 ppm, respectively, and a broad triplet of 6-H (VIIb), 8-H (VIIa and VIIb), and 5-H (VIIIa) methylene protons centered at 2.70 ppm are isolated in the PMR spectrum of the mixture in the strong-field region among a group of multiplets. The ratio of the sum of the areas of the methylidyne and methylene protons is 1:3, which corresponds to the theoretical

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*Here and subsequently, the m/e values of the ions are given.

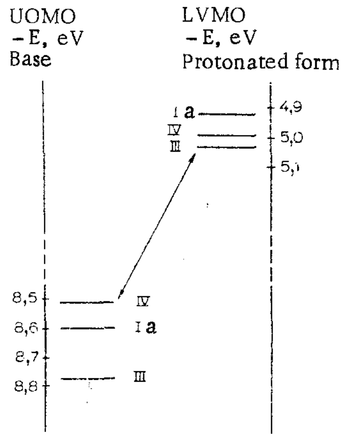

Fig. 1. Relative spacing of the levels of the LVMO and UOMO of Ia, III, and IV.

TABLE 4. Relative Intensities of the Peaks of the Characteristic Ions in the Mass Spectra of VIIa, b, VIIIa, and Xa, b

Compound	$\frac{I_{M-H}}{I_M}$	$\frac{I_{M-CH_3}}{I_M}$	$\frac{I_{M-C_2H_5}}{I_M}$	$\frac{I_{M-92}}{I_M}$	$\frac{I_{M-93}}{I_M}$	$\frac{I_{M-119}}{I_M}$	$\frac{I_{M-78}}{I_M}$	$\frac{I_{M-79}}{I_M}$
VIIIa	1,5	0,5	1,4	0,3	—	0,1		
VIIb	0,5	0,8	0,6	0,2	1,3	0,4		
VIIa	0,5	1,5	0,3	0,2	0,1	0,2		
Xa	1,2	0,6	1,1				0,2	—
Xb	0,7	0,2	0,5				0,4	0,7

value with allowance for the percentages of such of the components in the mixture. Signals of four α protons of the pyridine ring, of which one is in the form of a singlet at 8.16 ppm (1-H in VIIa, b), while the rest are in the form of doublets with a spin-spin coupling constant (SSCC) of 2 Hz at 8.09, 8.20, and 8.31 ppm (the α protons of the 6-methyl-2-pyridyl substituent, respectively, in VIIb, VIIa, and VIIIa), are observed in the weak-field region.

Thus in conformity with the theoretical calculations, processes involving cyclization with the participation of the 4 position of the pyridine ring (VIIa and VIIb) actually predominate in the dimerization of vinylpyridine II.

A comparison of the energy levels of the UOMO of the isomeric vinylpyridine bases and the LVMO of their protonated forms (Fig. 1) makes it possible to note that the highest-lying UOMO level belongs to the base IV molecule, while the lowest-lying LVMO level corresponds to protonated form III. This makes it possible to assume that "cross" cycloaddition in which β-vinylpyridine IV acts as the diene, and vinylpyridine III (in the protonated form) acts as the dienophile, should prevail in a mixture of these two compounds. A comparison of the energies of π-electron stabilization for all 12 theoretically possible regioisomers (Table 2) shows that the formation of Xa, Xb, and VI is most probable.

An equimolar mixture of vinylpyridines II and III was heated in glacial acetic acid at 130°C for 6 h, after which it was neutralized with Na_2CO_3 and analyzed by chromatographic mass spectrometry. Three compounds in a ratio of 1:11:7 were detected in the reaction mixture (in 60% overall yield). The identification of the substances obtained was simplified by the fact that the molecular mass of the dimer of vinylpyridine III is 210 and that of the dimer of vinylpyridine II is 238, while the molecular mass of the products of their cross reaction is 224. The molecular mass of the first of the compounds obtained is 210, and its retention time and mass spectrum coincide with the time and spectrum obtained for VI. The molecular mass of the other two compounds is 224. The peaks of [M—78] ions with mass 146 are present in the spectra of both compounds (Table 4), and this makes it possible to immediately exclude probable structures XIa, b. At the same time, the presence in the mass spectrum of the second of these compounds of intense peaks of [M—H] and [M—C_2H_5] ions makes it possible to assign the Xa structure to it, while the presence in the mass spectrum of the third compound of an intense peak of an [M—79] fragment with mass 145 similar to the [M—93] ion in the mass spectrum of VIIb makes it possible to assign the Xb structure to this compound.

Thus the actually observed regiospecificity of the cross dimerization is in good agreement with the regiospecificity predicted on the basis of quantum-chemical calculations.

EXPERIMENTAL

The PMR spectra of solutions of the compounds in CCl_4 were recorded with T-60 and XL-100 (Varian) spectrometers with hexamethyldisiloxane as the standard. The mass spectra of Va and VI were recorded with an MKh-1303 spectrometer with introduction of the substances into the ionization region at an ionizing-electron energy of 50 eV. The UV spectra of solutions of the compounds in methanol were recorded with a Cary-15 spectrophotometer. The chromatographic mass spectra were obtained with a MAT-111 (Varian) apparatus with a 1.5 m column (filled with 3% SE-30 on Chromosorb) with programmed heating with a thermostat from 150 to 250°C at a rate of 10 deg/min. The ionization energy was 80 eV.

The substances were isolated by preparative thin-layer chromatography on a 1.5-mm thick layer of aluminum oxide (activity II) in a benzene—methanol system (9:1).

Dimerization of 2-Vinylpyridines Ia-e. A solution of 0.2 mole of the corresponding vinylpyridine and 200 mg of hydroquinone in 50 ml of 85% phosphoric acid was added dropwise to 200 ml of heated (to 180-200°C) polyphosphoric acid (PPA) in the course of 2 h, after which the mixture was stirred thoroughly and heated for another 6 h. It was then cooled and poured with stirring over ice. The aqueous mixture was extracted with chloroform, and the extract was dried with anhydrous sodium sulfate. The chloroform was removed by distillation, and the residue was separated preparatively on aluminum oxide. 5-(2-Pyridyl)-5,6,7,8-tetrahydroquinolines Va-e (Table 3) were isolated from the bands with the R_f values indicated in Table 1.

8-(4-Pyridyl)-5,6,7,8-tetrahydroisoquinoline (VI). This compound was similarly obtained from 2.1 g (20 mmole) of 4-vinylpyridine. The yield was 1.7 g (80%). The bis(methiodide) had mp 172-174°C. UV spectrum, λ_{max} (log ε): 256 (3.7) and 290 nm (2.3). Mass spectrum, m/e (relative intensity, %): 210 (100), 209 (69), 195 (13), 182 (17), 181 (42), 132 (64), 130 (23), 118 (19), 117 (45), 106 (15), 78 (30). Found: C 79.9; H 6.6%. $C_{14}H_{14}N_2$. Calculated: C 80.0; H 6.7%.

Dimerization of 2-Methyl-5-vinylpyridine (II). The reaction and workup were carried out similarly. A mixture in an overall yield of 24% was isolated in the form of an oil from the band with R_f 0.31-0.33. UV spectrum, λ_{max} (log ε): 252 (4.0), 260 (4.0), and 266 nm(4.0). Found: C 80.5; H 7.5%. $C_{16}H_{18}N_2$. Calculated: C 80.7; H 7.6%.

6,7-Dimethyl-5-(2-pyridyl)-5,6,7,8-tetrahydroquinoline (Vf). A solution of 1.2 g (10 mmole) of trans-2-propenylpyridine (If) in 20 ml of PPA (containing no less than 93% phosphorus pentoxide) was heated in an autoclave at 350°C for 10 h, after which it was worked up as described above. Workup of the band with R_f 0.36-0.40 yielded 60 mg (5%) of Vf. UV spectrum, λ_{max} (log ε): 262 (3.9) and 268 nm (3.8). Mass spectrum, m/e (relative intensity, %): 238 (20), 233 (20), 195 (25), 183 (23), 182 (13), 181 (13), 169 (11), 120 (100), 107 (23), 106 (64), 93 (91). Found: C 80.5; H 7.6%. $C_{16}H_{18}N_2$. Calculated: C 80.7; H 7.6%.

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REACTION OF VINYLPYRIDINES WITH OXAZOLES

P. B. Terent'ev, N. P. Lomakina,
M. Islam Rakhimi, K. Dager Riad,
Ya. B. Zelikhover, and A. N. Kost*

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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 regiospecificity 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 regiospecificity 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 (IIId), 4-phenyl-5-methyloxazole (IIIe), 2-propyl-4-methyloxazole (IIIf), 2,4,5-trimethyloxazole

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*Deceased.

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

M. V. Lomonosov Moscow State University, Moscow 117234. Kabul Polytechnic Institute, Afghanistan. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 9, pp. 1255-1262, September, 1980. Original article submitted February 25, 1980.

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