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Synthesis and Structure of Indole-, Pyridine-, and Benzimidazole-Containing Nitroethenes

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Abstract — Previously unknown 2-(1,2-dimethylindol-3-yl)-1-nitroethene was synthesized, and procedures for preparing 2-(1-methylbenzimidazol-2-yl)- and 2-(3-pyridyl)-1-nitroethens were improved. The structures of the products were determined by spectroscopic methods and from their dipole moments. According to single crystal X-ray diffraction data, the (*E*)-2-(1-methylbenzimidazol-2-yl)-1-nitroethene molecules are virtually planar and are packed in stacks in the crystal lattice, with appreciable stacking interaction.

Compounds containing indole, pyridine, and benzimidazole fragments show biological activity [1] and widely occur in the nature. In particular, these fragments are present in molecules of many drugs: Indopan, Diazoline, Cordiamin, Dibasol, Furodazol, etc. [2]. Convenient synthetic precursors of compounds containing these pharmacophoric heterocycles are the corresponding 2-heteryl-1-nitroethenes. For example, aspidophytin alkaloid [3] and staurosporin, an active substance of some fungi [4], were prepared from indolylnitroethenes. 1-Nitro-2-(3-pyridyl)ethene and 1-nitro-2-(6-chloro-3-pyridyl)ethene are used in synthesis of pyrrolyzidine alkaloids [5], epibatidine alkaloid, and its analogs [6–9]. Indolylnitroethenes not only are interesting as synthetic precursors, but also exhibit amebicidal and fungicidal activity themselves [10, 11]. Therefore, optimization of the synthesis and study of structure and properties of the above-mentioned 2-heteryl-1-nitroethenes are urgent problems.

Unsaturated nitroalkanes are commonly prepared by reactions of nitroalkanes with aldehydes in the presence of base catalysts [12, 13]. We used this procedure to prepare 2-(indol-3-yl)- (**I**), 2-(1,2-dimethylindol-3-yl)- (**II**), 2-(3-pyridyl)- (**III**), and 2-(1-methylbenzimidazol-2-yl)-1-nitroethenes (**V**). In particular, compound **I** was prepared following the published protocol [14]; previously unknown compound **II** was prepared by the same procedure. However, we improved this general procedure by adding methanol to the hot reaction mixture after the reaction completion and then slowly cooling the mixture to room temperature with stirring. As a result, high-purity nitroalkenes **I** and **II** were isolated.

1-Nitro-2-(3-pyridyl)ethene **III** was prepared by condensation of nicotinaldehyde with nitromethane in the presence of methylamine [15, 16]. Modification of the procedures from [15, 16] (replacement of anhydrous ethanol by methanol) allowed the yield of the target product **III** to be increased from 55 to 73%, with high quality of the product.

2-(1-Methylbenzimidazol-2-yl)-1-nitroethene **V** was prepared according to [17]. In the first step, the reaction of 1-methyl-2-formylbenzimidazole with nitromethane in aqueous-alcoholic solution of NaOH afforded 2-(1-methylbenzimidazol-2-yl)-2-hydroxy-1-nitroethane **IV** in 65% yield. We obtained the first spectroscopic data for **IV** (see Experimental). The subsequent acylation of nitro alcohol **IV** with freshly distilled acetic anhydride under heating on a water bath for 3 min is accompanied by simultaneous deacylation and formation of the desired nitroethene **V**. However, when performed under these conditions (corresponding to the published protocol [17]), the mixture sometimes undergoes tarring, and no desired nitroalkene **V** is obtained. We improved this step of preparation of **V** from **IV** by changing the order of

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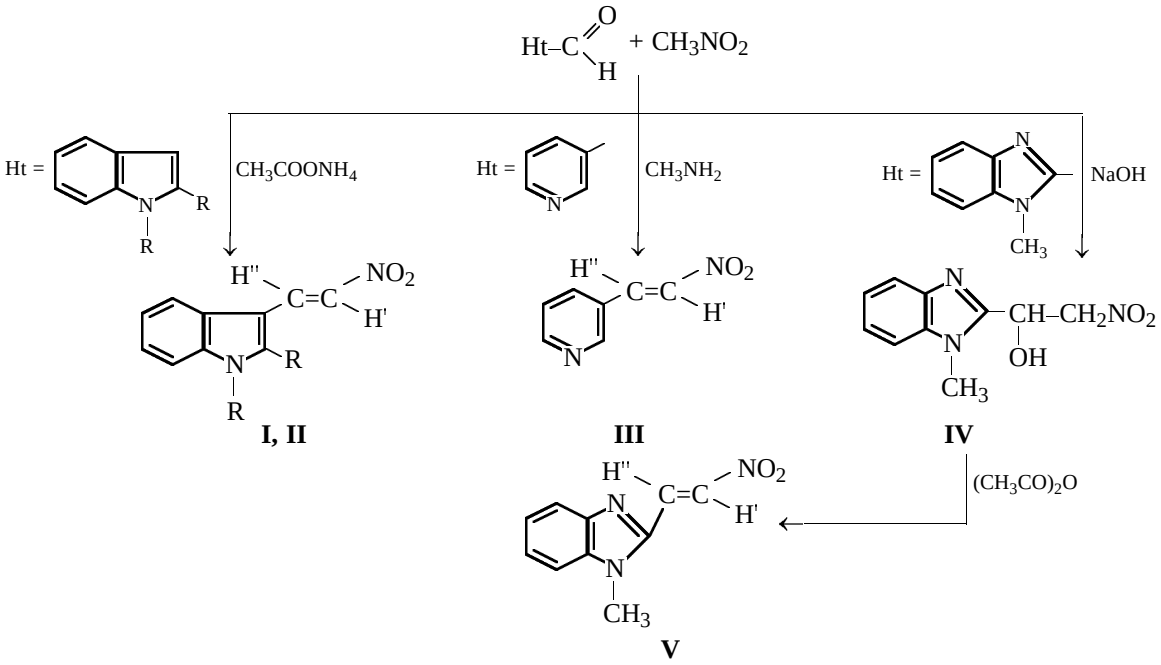


adding the reactants and by stirring the reaction mixture both in the course of heating and for 2 h after adding water to the reaction mixture. In this case, the tarring of **V** is prevented, and nitroalkene **V** is obtained in a reproducibly high yield, no less than 74%. All the heterylnitroethenes **I**–**III** and **V** are colored crystalline substances with well-defined melting points.

The structure of 2-(indol-3-yl)-1-nitroethene **I** was characterized [5, 18–23] by ^{1}H and ^{13}C NMR, IR, and UV spectroscopy, and also by single crystal X-ray diffraction, which allowed us to use this compound as reference. 1-Nitro-2-(3-pyridyl)ethene **III** was characterized by ^{1}H NMR spectroscopy, and the bond energies in its molecule were calculated in [15].

The characteristics of the ^{1}H NMR spectra of **II** and **V**, measured for the first time, are well consistent with the published data for 2-(indol-3-yl)-1-nitroethene **I** [5, 18–23] and 1-nitro-2-(3-pyridyl)ethene **III** [5, 15], respectively (Table 1). For example, in the ^{1}H NMR spectrum of **II**, the vicinal olefinic protons give an *AB* pattern with the signal centers at 7.75 (H') and 8.32 ppm (H'') and coupling constant of 13.4 Hz, typical of *trans*-protons. The indole ring protons in **II** give signals at 7.69–7.65 (1H), 7.32 (2H), and 7.28 ppm (1H); the methyl groups at C^2 and indole nitrogen atom give singlets at 2.57 and 3.77 ppm, respectively. In the ^{1}H NMR spectrum of 2-(1-methylbenzimidazol-2-yl)-1-nitroethene **V**, the olefinic protons also give an *AB* pattern with the signal centers at 7.97 (H') and 8.15 ppm (H'') and coupling constant of 13 Hz. The benzimidazole ring protons give two groups of low-field signals at 7.79 (1H) and 7.39 ppm (3H); the methyl protons give a singlet at 3.92 ppm (Table 1).

Table 1. ^{1}H NMR and electronic absorption[a] spectra of 2-heteryl-1-nitroethenes **II, III**, and **V**

Comp. no.	^{1}H NMR spectrum ($CDCl_3$), δ, ppm				Electronic absorption spectrum	
	H'	H''	Het	NCH_3 (CCH_3)	λ_{max}, nm	ε
II	7.75 d	8.32 d	7.69–7.65 m (1H, H^4), 7.28 s (1H, H^7), 7.32 s	3.77 s	225	20 600
	($^3J_{AB}$ 13.4 Hz)		(2H, H^5, H^6), 7.42 d.d (1H, H^5, ^3J 4.8, 7.7 Hz)	(2.57 s)	283	9700
					415	20 200
III	7.80 d	8.03 d	7.88 m (1H, H^4), 8.73 d.d (1H, H^6, ^{4+3}J 1.6,	–	219	16 700
	($^3J_{AB}$ 13.8 Hz)		4.8 Hz), 8.80 d (1H, H^2, ^4J 2.1 Hz)		294	19 200
V	7.97 d	8.15 d	7.39 s (3H), 7.79 m (1H)	3.92 s	212	16 700
	($^3J_{AB}$ 13 Hz)				361	17 200

[a] Solvent: **II**, acetonitrile; **III, IV**, methanol.

Table 2. IR data (ν, cm^{-1}) for **III** and **V**

Comp. no.	NO_2		CH=CH	
	ν_{as}	ν_s	ν	ν_{CH}
		CH_2Cl_2		
III	1528 s	1348 s	1640 m	972 m
V	1528 vs	1344 vs	1644 s	972 s
		Mineral oil		
III	1518 s	1352 s	1634 m	976 m
V	1526 s	1344 s	1646 s	974 s

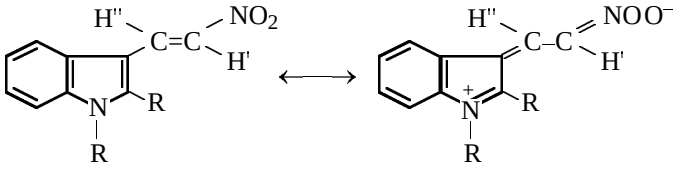
The ^1H NMR spectra of heterylnitroethenes **I**–**III** and **V** show that these compounds are stereochemically uniform and exist as *E* isomers. The medium-intensity IR bands at 972 (**II**) and 972–976 cm^{-1} (**III, V**), assignable to the CH out-of-plane bending vibrations in the CH=CH group, also suggest the *trans* orientation of the substituents in the molecules [24] (Table 2).

The IR spectra of **I**–**III** and **V** were taken from solid samples (mulls in mineral oil) and solutions in CH_2Cl_2 and $CHCl_3$. As seen from Table 2, in the spectra of **III** and **V** the absorption frequencies of the C=C bonds (1644–1634 cm^{-1}) and nitro groups (ν_{as} 1528–1518, ν_s 1352–1344 cm^{-1}) are typical of nitroethenes [18, 24].

The IR spectrum of **II**, as well as that of **I** [18, 23, 25–27], contains no bands of covalently bound nitro group but contains strong bands at 1310–1286 and 1284–1250 cm^{-1} assignable to the ionic nitro group and at 1500–1620 cm^{-1}, probably belonging to the system of conjugated multiple bonds with the prevalent contribution from $C=N^+$ [28–32]. The nicely consistent IR spectra of indolylnitroethenes **I** and **II** confirm the similarity of the fine structure of their molecules, and the specific features of the IR spectra reflect the high degree of polarization of the electron density in the indolylnitroethene moiety. This conclusion is consistent with the electronic absorption spectrum of **II**, containing a strong long-wave maximum at about 415 nm (Table 1), similar to that in the spectrum of **I** (λ_{max} 393 nm, ε 19429 l mol^{-1} cm^{-1}) [23]; hence, compound **II** is a highly conjugated system with a significant contribution of the bipolar structure. Such features of the IR and UV spectra of indole-containing nitroethenes **I** and **II**, compared to compounds **III** and **V**, are apparently due to more pronounced redistribution of the electron density in **I** and **II**, compared to pyridyl- and benzimidazolylnitroethenes **III** and **V**.

The same conclusion follows from the experimental dipole moments of heterylnitroalkenes **I**–**III** and **V** (Table 3). For example, the dipole moment of **II**, measured in dioxane, is higher than that of **V** by 2.22 D (Table 3).

Furthermore, for indole-substituted nitroethenes **I**



I, II

R = H (**I**), CH_3 (**II**).

Table 3. Coefficients of calculation equations, orientation polarizations, and calculated and experimental dipole moments of **I**–**III** and **V**

Comp. no.	Solvent	α	γ	P_{or}, cm^3	μ_{exp}, D	μ_{calc}, D	
						E isomer	*Z* isomer
I	Benzene	26.010	1.451	868.023	6.52	4.18	3.30
II	"	26.802	0.787	1056.637	7.19	4.63	3.20
	Dioxane	33.844	0.797	1173.830	7.58		
III	Benzene	10.547	0.353	287.536	3.75	4.32	3.27
	Dioxane	14.824	2.471	299.357	3.83		
V	"	18.371	0.796	586.721	5.36	6.15	3.32

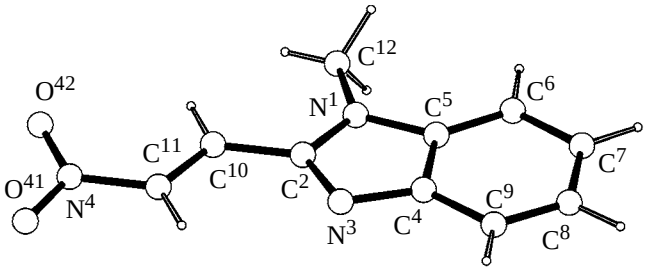


Fig. 1. Geometry of the molecule of **V** in the crystal.

and **II**, $\Delta\mu$ between the experimental (in benzene) and calculated (for *E* isomers) dipole moments is 2.34 and 2.56 D, respectively, which also suggests significant redistribution of the electron density in molecules of indolylnitroethenes **I** and **II** between the donor heterocycle and acceptor nitro group. For **III** and **V**, $\Delta\mu$ is considerably smaller (0.49 and 0.79 D) and has different sign, which also suggests considerably weaker polarization of molecules of nitroethenes **III** and **V**, compared to **I** and **II**.

When calculating the dipole moments, we used the following moments of bonds and groups: $m(H\rightarrow C_{sp^2})$ 0.7 [33], $m(C_{sp^2}–NO_2)$ 2.81 D {calculated from $\mu_{exp}(CH_2=CHNO_2)$ [34]}. The group moment of the pyridine ring (1.51 D) was calculated from μ_{exp} of pyridine [34]; that of the indole ring (1.37 D), from μ_{exp} of indole [34]; that of the 1,2-dimethylindole ring (1.82 D), from μ_{exp} of 1,2-dimethylindole [34]; and that of the 1-methylbenzimidazole ring (3.34 D), from μ_{exp} of *N*-methylbenzimidazole [34]. The direction of the group moments of nitrogen-containing heterocycles is from the heterocycle to C_{sp^2}. In calculations, we used the bond angles determined in a single crystal X-ray diffraction study of 2-(1-methylbenzimidazol-2-yl)-1-nitroethene **V** ($\angle C=CH^1$ 118°, $\angle C=CH^2$ 117°, $\angle NO_2C=C$ 121°, $\angle C=CC$ 122°).

According to single crystal X-ray diffraction data, the 2-(1-methylbenzimidazol-2-yl)-1-nitroethene molecule in the crystal is virtually planar, with the *trans* configuration at the double bond (Fig. 1). The steric structure of **V** is shown in Figs. 1–3, and the atomic coordinates and geometric parameters are listed in Tables 4 and 5. The oxygen atoms of the nitro group show the largest deviation from the least-squares plane of the molecules [maximal deviation 0.145(5) Å]. Without considering the oxygen atoms of the nitro group and the methyl carbon atom, the molecule is planar to within 0.027(5) Å. Thus, the double bond and the benzimidazole fragment can form a common conjugated system. The bond length distribution is consistent with this assumption. The molecules in the crystal are packed in stacks in the antiparallel fashion

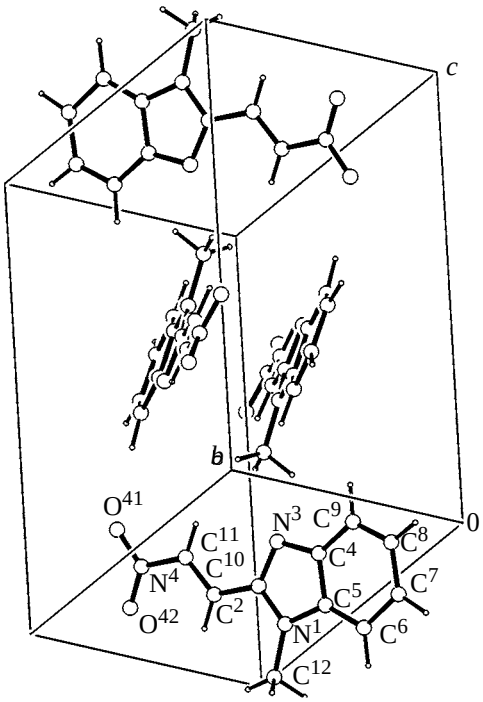


Fig. 2. Unit cell of the crystal of **V**.

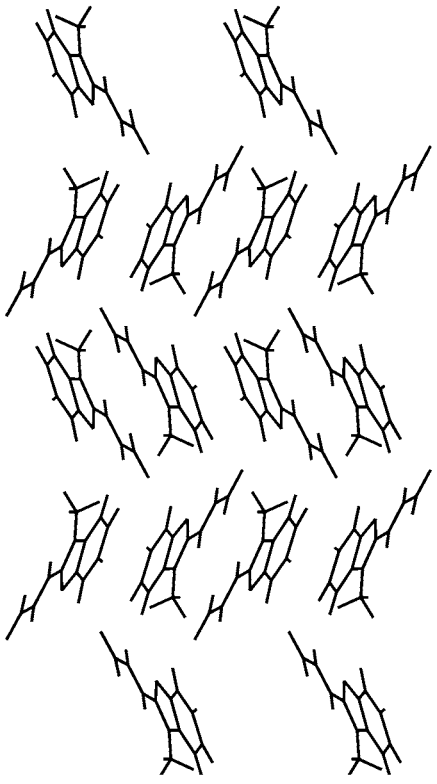


Fig. 3. Molecular packing of **V** in the crystal.

(Figs. 2, 3). A short contact of 3.31 Å between the planes of the benzimidazole fragment in the stacks suggests the occurrence of stacking interaction in the crystal.

Table 4. Atomic coordinates in the structure of **V**, equivalent isotropic temperature factors of nonhydrogen atoms $B = 4/3 \sum_{i=1}^{3} \sum_{j=1}^{3} (a_i a_j) B(i, j)$ (Å^2), and isotropic temperature factors of hydrogen atoms B_{iso} (Å^2)

Atom	*x*	*y*	*z*	B_{iso}
O^{41}	0.9646(4)	0.6275(6)	1.2627(3)	7.6(1)
O^{42}	1.0302(4)	0.5289(7)	1.1246(3)	8.0(1)
N^1	0.5842(4)	0.2649(5)	0.9570(3)	3.69(7)
N^3	0.5247(4)	0.3333(5)	1.1102(3)	3.89(8)
N^4	0.9410(4)	0.5511(5)	1.1810(3)	4.48(9)
C^2	0.6235(5)	0.3351(6)	1.0474(4)	3.72(9)
C^4	0.4158(4)	0.2552(6)	1.0538(3)	3.56(8)
C^5	0.4487(5)	0.2087(5)	0.9563(4)	4.1(1)
C^6	0.3606(6)	0.1266(7)	0.8840(5)	5.6(1)
C^7	0.2275(7)	0.0890(7)	0.9143(6)	7.8(2)
C^8	0.1930(6)	0.1402(8)	1.0110(5)	6.3(1)
C^9	0.2818(5)	0.2206(8)	1.0789(4)	5.5(1)
C^{10}	0.7629(5)	0.4038(6)	1.0712(3)	4.4(1)
C^{11}	0.8031(5)	0.4827(7)	1.1592(4)	4.4(1)
C^{12}	0.6607(6)	0.2552(9)	0.8682(4)	6.5(1)
H^6	0.390(9)	0.09(1)	0.815(8)	7(3)
H^7	0.164(6)	0.032(9)	0.856(5)	10(2)
H^8	0.10(1)	0.12(2)	1.02(1)	8(4)
H^9	0.26(2)	0.25(3)	1.15(2)	8(4)
H^{10}	0.830(9)	0.39(1)	1.022(7)	5(3)
H^{11}	0.734(7)	0.49(1)	1.207(6)	5(3)
H^{121}	0.747(5)	0.294(6)	0.868(4)	9(4)
H^{122}	0.65(2)	0.13(3)	0.84(2)	8(4)
H^{123}	0.604(7)	0.321(9)	0.806(6)	9(4)

Comparative analysis of the single crystal X-ray diffraction data for **V** (this work) and **I** [23] confirms the above conclusions. In particular, the C–NO_2 (1.433 Å) and C–Ht (1.451 Å) bonds in **V** are appreciably longer than in **I** (1.424 and 1.422 Å, respectively), suggesting weaker conjugation in **V**.

Thus, we have prepared previously unknown 2(1,2-dimethylindol-3-yl)-1-nitroethene and optimized the procedures for preparing its pyridine- and 1-methylbenzimidazole-containing analogs. The fine structure of these molecules was studied by the method of dipole moments, ^{1}H NMR, IR, and UV spectroscopy, and single crystal X-ray diffraction. Comparative analysis of the physicochemical characteristics described for the reference compound, 1-(indol-3-yl)-2-nitroethene **I**, with those obtained for heterylnitroethenes **II**, **III**, and **V** suggests that all these nitroethenes are *E* isomers; indole-containing nitroethenes **I** and **II** are highly conjugated systems with a significant contribution of the bipolar structure. According to single crystal X-ray diffraction, the molecules of (*E*)-2-(1-methylbenzimidazol-2-yl)-1-nitroethene are virtually planar and are packed in stacks in the crystal, with the stacking interaction.

Table 5. Principal geometric parameters of the structure of **V**: bond lengths (*d*, Å), bond angles (ω, deg), and torsion angles (τ, deg)

Bond	*d*	Bond	*d*
O^{41}–N^4	1.228(6)	C^2–C^{10}	1.451(7)
O^{42}–N^4	1.220(6)	C^4–C^5	1.412(7)
N^1–C^2	1.328(6)	C^4–C^9	1.405(7)
N^1–C^5	1.382(6)	C^5–C^6	1.360(7)
N^1–C^{12}	1.466(7)	C^6–C^7	1.426(9)
N^3–C^2	1.341(6)	C^7–C^8	1.42(1)
N^3–C^4	1.358(5)	C^8–C^9	1.321(8)
N^4–C^{11}	1.433(6)	C^{10}–C^{11}	1.331(7)
Angle	**ω**	**Angle**	**ω**
$C^2N^1C^5$	107.6(4)	$N^3C^4C^9$	129.3(4)
$C^2N^1C^{12}$	128.8(4)	$C^5C^4C^9$	119.0(4)
$C^5N^1C^{12}$	123.4(4)	$N^1C^5C^4$	103.5(4)
$C^2N^3C^4$	103.3(4)	$N^1C^5C^6$	131.8(5)
$O^{41}N^4O^{42}$	122.3(4)	$C^4C^5C^6$	124.8(5)
$O^{41}N^4C^{11}$	115.0(4)	$C^5C^6C^7$	114.1(6)
$O^{42}N^4C^{11}$	122.6(4)	$C^6C^7C^8$	121.2(5)
$N^1C^2N^3$	113.9(4)	$C^7C^8C^9$	122.7(6)
$N^1C^2C^{10}$	120.2(4)	$C^4C^9C^8$	118.2(5)
$N^3C^2C^{10}$	125.8(4)	$C^2C^{10}C^{11}$	121.6(5)
$N^3C^4C^5$	111.7(4)	$N^4C^{11}C^{10}$	120.8(5)
Angle	**τ**	**Angle**	**τ**
$C^5N^1C^2N^3$	–0.5(5)	$O^{41}N^4C^{11}C^{10}$	177.1(5)
$C^5N^1C^2C^{10}$	179.1(4)	$O^{42}N^4C^{11}C^{10}$	–5.8(7)
$C^{12}N^1C^2N^3$	175.5(5)	$N^1C^2C^{10}C^{11}$	176.6(4)
$C^{12}N^1C^2C^{10}$	–5.0(7)	$N^3C^2C^{10}C^{11}$	–3.9(7)
$C^2N^1C^5C^4$	0.5(5)	$N^3C^4C^5N^1$	–0.4(5)
$C^2N^1C^5C^6$	–179.0(5)	$N^3C^4C^5C^6$	179.1(4)
$C^{12}N^1C^5C^4$	–175.7(4)	$C^9C^4C^5N^1$	178.4(4)
$C^{12}N^1C^5C^6$	4.8(8)	$C^9C^4C^5C^6$	–2.1(7)
$C^4N^3C^2N^1$	0.2(5)	$N^3C^4C^9C^8$	–179.2(5)
$C^4N^3C^2C^{10}$	–179.4(4)	$N^1C^5C^6C^7$	179.4(5)
$C^2N^3C^4C^5$	0.2(5)	$C^2C^{10}C^{11}N^4$	–179.5(4)
$C^2N^3C^4C^9$	–178.5(5)		

EXPERIMENTAL

The ^{1}H NMR spectra were recorded on a Bruker AC-200 spectrometer (200 MHz) in chloroform-*d* (**II**, **III**, **V**) or acetonitrile-d_3 (**IV**), internal reference

HMDS. The IR spectra were recorded on a Specord M-80 spectrophotometer [mulls in mineral oil (**I**–**III**, **V**), solutions in dichloromethane (**I**–**III**, **V**), or KBr pellets (**IV**). The electronic absorption spectra were measured on an SF-121 spectrophotometer in acetonitrile (**I**, **II**) or methanol (**III**, **V**).

Crystals of 2-(1-methylbenzimidazol-2-yl)-1-nitroethene **V**, $C_{10}N_9N_3O_2$, are monoclinic. The unit cell parameters at 20°C are as follows: *a* 9.715(4), *b* 7.632(3), *c* 13.261(9) Å; β 96.65(5)°, *V* 976.6(9) Å^3, *Z* 4, d_{calc} 1.38 g cm^{-3}, space group $P2_1/c$. The unit cell parameters and intensities of 2278 reflections, including 1037 reflections with $I \geq 3\sigma$, were measured on an Enraf–Nonius CAD-4 automatic four-circle diffractometer ($\lambda Cu K_\alpha$ radiation, graphite monochromator, $\omega/2\theta$ scanning, $\theta \leq 76.9°$). No decrease in the intensity of three check reflections within the time of measurements was observed. The absorption (μCu 7.91 cm^{-1}) was not taken into account. The structure was solved by the direct method using the SIR program [35] and refined first in the isotropic and then in the anisotropic approximation. The methyl hydrogen atoms were revealed from the differential electron density syntheses, and the other hydrogen atoms were placed in the calculated positions. Their contribution to the structural amplitudes was taken into account with fixed positional and isotropic thermal parameters. The final divergence factors were *R* 0.069, R_W 0.074 for 686 unique reflections with $F^2 \geq 3\sigma$. All the calculations were performed on an AlphaStation-200 computer using MolEN program package [36]. The intermolecular interactions were analyzed and the structures plotted with the PLATON program [37].

The dipole moments of **I**–**III** were determined in benzene, and those of **II**, **III**, and **V**, in dioxane at 25°C with an IDM-2 device according to [38]. The orientation polarizations and coefficients of the calculation equations are given in Table 3.

1-Methylbenzimidazole-2-carbaldehyde was prepared according to [39], and 2-(indol-3-yl)-1-nitroethene **I**, by the modified procedure in [14]. Commercial nicotinaldehyde was used.

2-(1,2-Dimethylindol-3-yl)-1-nitroethene II. A mixture of 20 ml of nitromethane, 1.54 g of ammonium acetate, and 7 g of 1,2-dimethylindole-3-carbaldehyde was refluxed with continuous stirring for 30 min, after which 17.6 ml of 60% aqueous methanol was added, and the mixture was cooled to 5°C. The crystalline precipitate was filtered off. Yield 6.3 g (73%), mp 170°C (from methanol). Found, %: C 66.76, 66.75; H 5.68; 5.64; N 12.93; 12.95. $C_{12}H_{12}N_2O_2$. Calculated, %: C 66.67; H 5.56; N 12.96.

1-Nitro-2-(3-pyridyl)ethene III. To a mixture of 10 ml of methanol and 15 ml of nitromethane, we added with stirring 0.4 g of methylamine hydrochloride, 0.2 g of sodium hydrogen carbonate, and 10.7 ml of nicotinaldehyde. The mixture was stirred for 72 h. The precipitate was filtered off and washed with a small amount of methanol. Yield of **III** 11 g (73%); mp 138–140°C (from methanol) (published data: mp 140°C [16]). Found, %: C 56.55, 56.55; H 4.52, 4.51; N 18.41, 18.39. $C_7H_6N_2O_2$. Calculated, %: C 56.00; H 4.00; N 18.67.

2-(1-Methylbenzimidazol-2-yl)-2-hydroxy-1-nitroethane IV was prepared according to [17]. IR spectrum (KBr), ν, cm^{-1}: 1384, 1560 (NO_2); 3650–3300 (OH). ^{1}H NMR spectrum (CD_3CN), δ, ppm: 5.15–4.96 m (CH_2), 5.69–5.63 m (CH), 7.61 d (1H-Bz), 7.48 d (1H-Bz), 7.34–7.19 m (2H-Bz), 3.85 s (NCH_3).

2-(1-Methylbenzimidazol-2-yl)-1-nitroethene V. To 5 ml of acetic anhydride, we added with stirring 2.2 g of 2-(1-methylbenzimidazol-2-yl)-2-hydroxy-1-nitroethane **IV**. The mixture was heated on a boiling water bath until the precipitate fully dissolved (3–4 min). Then 40 ml of ice-cold water was added, and the mixture was stirred for 2 h. The yellow crystalline product was filtered off and washed on the filter with water, alcohol, and ether. Yield of **V** 1.5 g (74%), mp 137–139°C (from methanol) {published data: mp 139–140°C (methanol) [17]}. Found, %: C 59.15, 59.18; H 4.53; 4.50; N 20.70; 20.63. $C_{10}H_9N_3O_2$. Calculated, %: C 59.11; H 4.46; N 20.68.

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