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β,β-Dinitrostyrenes: Specificity of Synthesis and Structure

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Abstract—An improved procedure was developed for the synthesis of β,β-dinitrostyrenes, which increased the yield and reproducibility and made the products more accessible from the preparative viewpoint. Complex analysis of the spectral data (IR, UV, ^{1}H and ^{13}C NMR) and results of quantum-chemical calculations showed that 2-aryl-1,1-dinitroethene molecules have a structure in which one nitro group resides in the C=C bond plane while the other deviates from this plane. The C=C bond in 2-aryl-1,1-dinitroethene molecules was found to possess enhanced polarization and electrophilicity as compared to the corresponding bond in model mononitrostyrenes.

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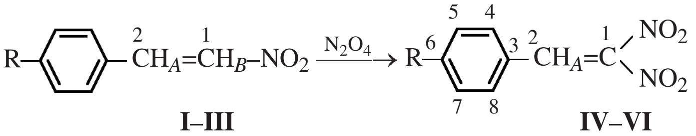
Conjugated nitro alkenes attract increased interest as convenient models for studying general theoretical problems of organic chemistry, as well as starting compounds for the synthesis of practically important substances (drugs, pesticides, analogs of naturally occurring compounds, energetic materials, etc.) [1–3]. In particular, just β-nitrostyrene was the key compound in the first synthesis of Fenibut, a novel nontoxic nootropic agent used in medical practice [4, 5].

Introduction of the second nitro group into mononitroethene molecules enhances electrophilicity of the double C=C bond thus giving rise to qualitatively new highly reactive compounds [6–8]. Typical representatives of this series are geminal dinitrostyrenes that are convenient models for studying specificity of the effect of two nitro groups on the reactivity of the double bond in comparison with mononitrostyrenes and their derivatives containing a different substituent (halogen atom, acetyl group, etc.) at the same carbon atom. In this connection, we thought it to be expedient to examine in detail the structure of β,β-dinitrostyrenes with a view to elucidate their synthetic potential as starting materials for purposeful preparation of functionally substituted structures.

Geminal dinitrostyrenes **IV**–**VI** were prepared according to improved procedures [6, 7] by nitration of the corresponding mononitrostyrenes **I**–**III** with almost tenfold excess of dinitrogen tetraoxide in carbon tetrachloride at 16–18°C.



I–**III** **IV**–**VI**

I, IV, R = H; **II, V**, R = Cl; **III, VI**, R = CH_3.

After removal of the solvent and excess nitrating agent, the mixture was treated with propan-2-ol at 16–18°C instead of ethanol at –5°C as recommended in [7]. It is known that ethanol adds to β,β-dinitrostyrenes at room temperature almost instantaneously [8], while low-temperature treatment complicates the experimental procedure. The use of propan-2-ol at room temperature allowed us to simplify isolation of the resulting dinitrostyrenes, improve their yield (from 42.5 to 79% for compound **IV** and from 39.5 to 49% for **V**), and made the procedure readily reproducible and preparatively accessible (Table 1).

Table 1. Yields and IR, UV, and ^1H and ^{13}C NMR spectra of β,β-dinitrostyrenes **IV**–**VI** and β-nitrostyrenes **I**–**III**

Comp. no.	Yield (published data), %	IR spectrum, ($CHCl_3$), ν, cm^{-1}		UV spectrum ($CHCl_3$)		NMR spectra ($CDCl_3$), δ, ppm			
						^1H		^{13}C	
		NO_2 [a] (Δν)	C=C, Ar	λ_{max}, nm	ε	H_A (H_B)	Ar	C^1	C^2
I		1530, 1345 (185)	1645	243 313	5400 17 900	7.87 (7.60)	7.38	137.1	138.9
IV	79 (42.5)	1550, 1320 (230)	1610 1650	244 324	8600 17 200	8.03	7.47–7.68	149.0	127.2
II		1525, 1340 (185)	1630	242 328	11 800 31 600	7.75 (7.47)	7.37	137.5	137.7
V	49 (39.5)	1550, 1320 (230)	1600 1645	245 342	20 100 40 000	7.98	7.39–7.55	149.2	126.2
III		1520, 1340 (180)	1630	244 328	8300 21 000	7.95 (7.54)	7.33	136.3	139.1
VI [b]	65 (65)	1550, 1320 (230)	1610 1640	242 341	10 800 23 400	7.96	7.27–7.45	148.9	127.5

[a] Broadened bands. [b] Chemical shifts of the CH_3 group: δ 2.46 ppm, δ_C 21.6 ppm.

We thus obtained a series of β,β-dinitrostyrenes, including those having electron-withdrawing (Cl) and electron-donor substituents (CH_3) in the para position of the benzene ring and no substituent therein. It should be noted that the melting point of a sample of **VI** isolated by us (70–71°C) considerably differed from the melting point given in [7] (52–54°C); presumably, the latter is invalid, for the structure of our sample was reliably confirmed by independent methods (IR, UV, and ^1H and ^{13}C NMR spectra).

Aryldinitroethenes **IV**–**VI** are light yellow crystalline substances that are fairly stable. They can be stored for 1–1.5 month at room temperature, and then slow decomposition begins. To prolong their lifetime, compounds **IV**–**VI** should be stored at reduced temperature. It should be noted that the simplest representative of this series, 1,1-dinitroethene, was not isolated individual; it is generated in situ from appropriate functionally substituted precursors [9–11].

The structure of geminal dinitrostyrenes **IV**–**VI** was studied by spectral methods (1H and ^{13}C NMR, IR, UV) and quantum-chemical calculations (B3LYP/6-31+G*) with a view to analyze specificity of their structure as compared to mononitrostyrene.

The IR spectra of β,β-dinitrostyrenes **IV**–**VI** contain strong broadened absorption bands typical of conjugated nitro group (1550 and 1320 cm^{-1}) and bands belonging to stretching vibrations of the C=C bond and aromatic ring (1600–1610, 1640–1650 cm^{-1}; Table 1). The difference between the frequencies of antisymmetric and symmetric vibrations of the nitro groups in compounds **IV**–**VI** is $\nu_{as} - \nu_s = \Delta\nu \approx 230\ cm^{-1}$, which is typical of geminal dinitrostyrenes [12]; the corresponding difference for mononitrostyrenes is 180–185 cm^{-1}.

The electronic absorption spectrum of the simplest β,β-dinitrostyrene (**IV**) in cyclohexane was reported in [13]: λ_{max1} 224 nm (ε = 8415), λ_{max2} 313 nm (ε = 15 850) [13]; only the positions of long-wave absorption maxima in the spectra of **V** and **VI** in dioxane were given in [7]: λ_{max} 329 and 334 nm, respectively. Comparison of the electronic absorption spectra of dinitrostyrenes **IV**–**VI** in chloroform (λ_{max1} 242–245 nm, λ_{max2} 324–342 nm) with those of β-nitrostyrenes (λ_{max1} 242–244 nm, λ_{max2} 313–328 nm) [13] shows that introduction of the second nitro group induces a small red shift ($\Delta\lambda_{max2} \approx 13$ nm) of the long-wave absorption band (Table 1). A red shift of the long-wave absorption maximum (≈ λ 17 nm) is also observed in going from compound **IV** to **V** and **VI** where the substituent exerts mesomeric of hyperconjugation effect.

The ^1H NMR parameters of β,β-dinitrostyrenes **IV**–**VI** [δ 7.96–8.03 (CH_A), 7.27–7.68 ppm (H_{arom})] almost coincide with those reported for 1,1-dinitro-2-phenylethene [$CDCl_3$: δ 8.00 (CH_A), 7.49 ppm (H_{arom})] [14] and are close to the corresponding parameters of 2-nitro-3-phenylacrylonitrile [δ 7.83 (CH_A), 6.65–

Table 2. Bond angles ω (deg) in molecules **I** and **IV**–**VI**

Comp. no.	$C^3C^2C^1$	$C^2C^1N^9$	$C^2C^1N^{12}$	$N^9C^1N^{12}$
IV	131.9	121.9	125.9	112.2
V	131.6	121.9	125.8	112.2
VI	131.9	122.0	125.8	112.2
I	126.9	120.6	–	–

7.45 ppm (H_{arom})] [14]. It is important that the olefinic protons in **IV**–**VI** resonate in a weaker field (δ 7.83–8.03 ppm) than the aromatic protons (δ 6.65–7.68 ppm). Undoubtedly, joint deshielding effect of two nitro groups is responsible for the more downfield position of the olefinic proton signals of β,β-dinitrostyrenes relative to the corresponding signals of mononitrostyrenes (δ 7.47–7.60 ppm) (Table 1).

The ^{13}C NMR spectra of **IV**–**VI**, recorded without decoupling from protons, contain a strong doublet signal from C^2 at δ_C 126.2–127.5 ppm (J_{CH} = 162.8 Hz) and a downfield singlet at δ_C 148.9–149.2 ppm due to resonance of the C^1 nuclei; signals from aromatic carbon nuclei appear in the region δ_C 122.5–145.8 ppm (Table 1). It is seen that β,β-dinitrostyrenes are characterized by more downfield position of the C^1 signal (δ_C 148.9–149.2 ppm) as compared to mononitrostyrenes (Table 1), which results from deshielding effect produced by two nitro groups. It should be noted that the resonance signals of C^1 are broadened due to coupling with quadrupolar ^{14}N nuclei [15–18].

To estimate the degree of polarization and elucidate electronic and steric structure of compounds **IV**–**VI** we performed quantum-chemical calculations of geometric parameters of their molecules, dipole moments, and charges on atoms using Gaussian 03w software package [19] in terms of the density functional theory [20] (B3LYP/6-31+G*) with account taken of diffuse and polarization functions. Analogous calculations were also performed for 1-nitro-2-phenylethene (**I**) as model structure, The principal geometric parameters of molecules **I** and **IV**–**VI** are given in Tables 2–4, and the molecular models are shown in figure.

It is seen that the plane of one of the nitro groups considerably declines from the plane of the arylnitroethene fragment. The torsion angles $C^3C^2C^1N^9$, $C^2C^1N^9O^{10}$, and $C^2C^1N^9O^{11}$ in molecules **I** (180.0, 180.0, and 0.0°, respectively) and **IV**–**VI** (179.7–180.0, 178.2–178.7, and 1.1–1.5°, respectively; Tables 2, 3) indicate planar structure of the arylnitroethene fragment. On the other hand, the torsion angles $C^3C^2C^1N^{12}$ (–0.5 to –0.9°), $C^2C^1N^{12}O^{13}$ (85.0 to 86.3°), $C^2C^1N^{12}O^{14}$ (–92.0 to –93.3°), $N^9C^1N^{12}O^{13}$ (–94.8 to –95.7°) and $N^9C^1N^{12}O^{14}$ (85.9 to 86.9°) in β,β-dinitrostyrene molecules correspond to almost orthogonal orientation of the second nitro group with respect to the arylnitroethene fragment. Therefore, interaction of between the second nitro group and the C=C bond is weakened.

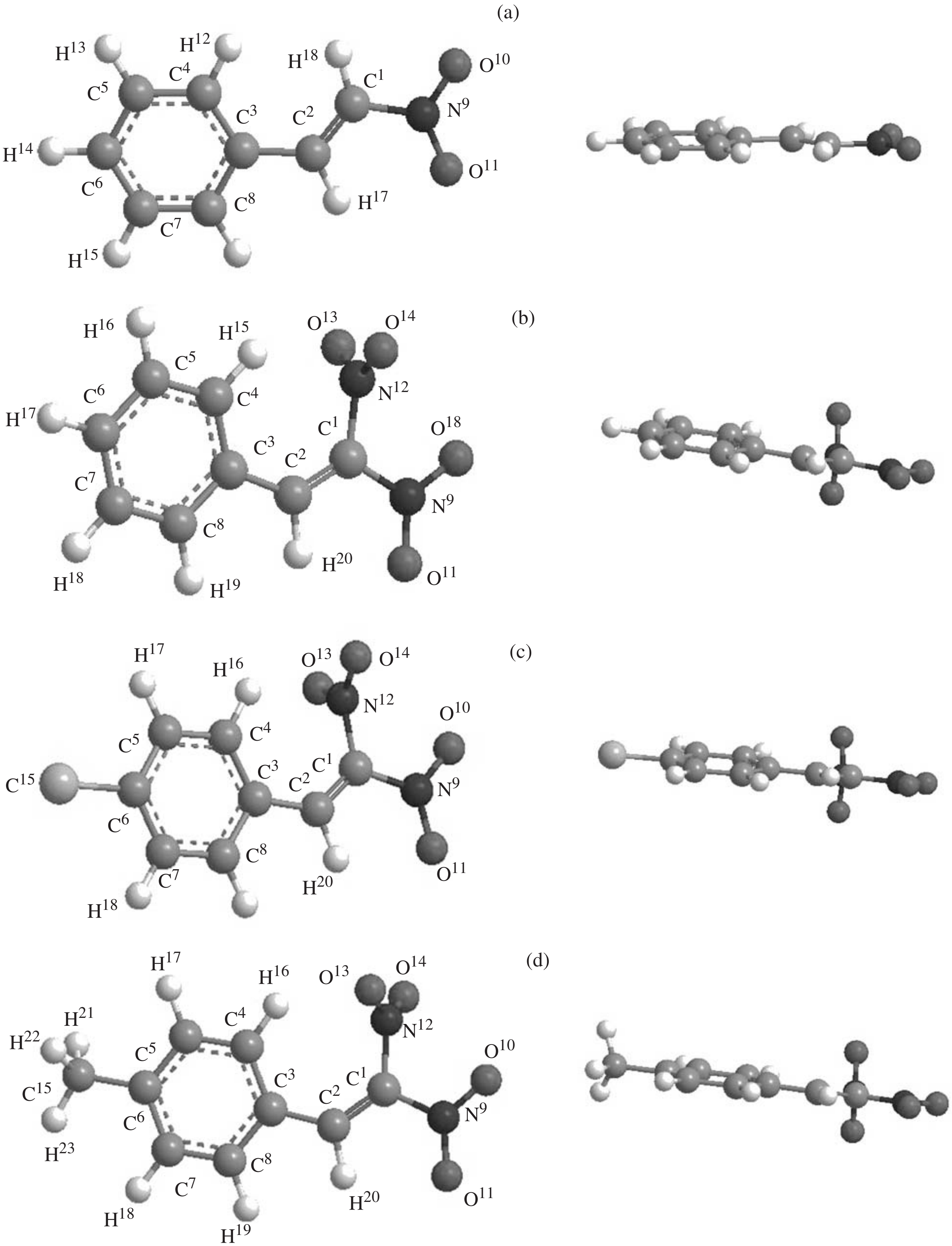
According to the calculations, the C^1=C^2 bond length (Table 4) almost does not change in going from mononitrostyrene to geminal dinitrostyrene, and it remains similar to the C=C bond length in nitroethene and its monosubstituted analogs (1.34–1.32 Å) [21–29]. The C^1–N^9 bond length in β,β-dinitrostyrenes **IV**–**VI** (1.455–1.458 Å) is close to that in β-nitrostyrene. However, this bond in molecules **I** and **IV**–**VI** is shorter than in nitroethene (1.451 Å for **I** against 1.470 Å in nitroethene [21]); undoubtedly, the reason is extension of the conjugation system due to the presence of phenyl substituent.

The difference between the lengths of the C^1–N^9

Table 3. Torsion angles τ (deg) in molecules **I** and **IV**–**VI**

Comp. no.	$C^3C^2C^1N^9$	$C^3C^2C^1N^{12}$	$C^2C^1N^9O^{10}$	$C^2C^1N^9O^{11}$
IV	–179.8	–0.7	–178.2	1.5
V	–179.7	–0.9	–178.7	1.1
VI	–180.0	–0.5	–178.2	1.5
I	–180.0	–	–180.0	–0.008

Comp.	$C^2C^1N^{12}O^{13}$	$C^2C^1N^{12}O^{14}$	$N^9C^1N^{12}O^{13}$	$N^9C^1N^{12}O^{14}$
IV	85.1	–93.2	–95.7	85.9
V	86.3	–92.0	–94.8	86.9
VI	85.0	–93.3	–95.6	86.2



Molecular models of (a) 1-nitro-2-phenylethene (**I**), (b) 1,1-dinitro-2-phenylethene (**IV**), (c) 2-(*p*-chlorophenyl)-1,1-dinitroethene (**V**), and (d), 1,1-dinitro-2-(*p*-tolyl)ethene (**VI**), calculated at the B3LYP/6-31+G* level.

Table 4. Bond lengths *d* (Å) in molecules **I** and **IV**–**VI**

Comp. no.	C^1=C^2	C^1–N^9	C^1–N^{12}
IV	1.343	1.458	1.474
V	1.342	1.458	1.474
VI	1.344	1.455	1.474
I	1.343	1.451	–

Table 5. Calculated charges on the C^1 and C^2 atoms and dipole moments of compounds **IV**–**VI**

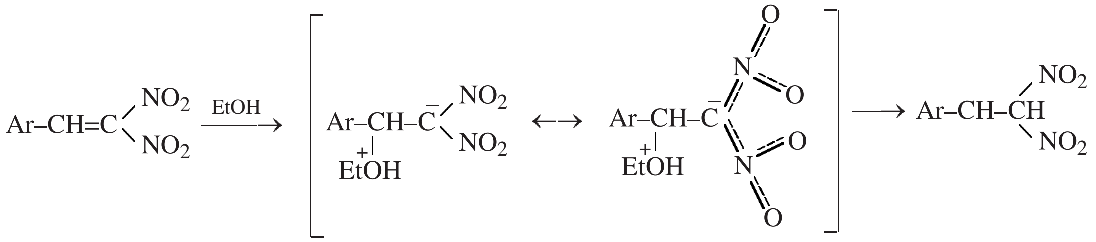
Comp.	Charge (NBO)		μ, D	
	C^1	C^2	calculated[a]	experimental [13, 33]
IV	0.192	–0.150	7.12	5.28
V	0.194	–0.154	5.71	–
VI	0.188	–0.149	8.04	–
I	–0.110	–0.160	6.36	4.32

[a] B3LYP/6-31+G*.

(1.455–1.458 Å) and C^1–N^{12} bonds (1.474 Å) must be noted. It seems to be expected taking into account that the second nitro group (N^{12}) interacts with the double bond less effectively than does the first nitro group (N^9). The C^1–N^{12} bond length (1.474 Å) approaches those found in 1-acetyl-1-nitro-2-(*p*-methoxyphenyl)ethene (1.476 Å) and 1-nitro-2-(*p*-nitrophenyl)-1-ethoxycarbonylethene (1.472 Å) [30], where the nitro group is also forced out of the double bond plane.

Effective charges on atoms (*q*) are parameters that characterize electronic structure of molecules. We used natural charges. Analysis of the populations calculated in the B3LYP/6-31+G(d) approximation was performed in terms of the NBO approach (Natural bond orbitals, Version 3.1, Gaussian-03w) [31]. Natural charges reproduce electron density distribution more accurately than total Mulliken charges [32]. The calculations showed that introduction of the second nitro group reduces the negative charge on C^2, the charge on C^1 changes correspondingly (Table 5). The calculated charges on the double-bonded carbon atoms correlate with the ^{13}C NMR data [17]. Contrasting charge distribution and strong difference in the chemical shifts of C^1 and C^2 ($\Delta\delta_C = \delta_{C^1} - \delta_{C^2}$) are responsible for the high dipole moments. Although the calculated and experimental dipole moments [13, 33] differ considerably, the character of their variation in going from mono- to dinitrostyrenes is the same: the dipole moment increases (Table 5).

Our results suggest that the C=C bond in geminal dinitrostyrenes is strongly electron-deficient and that the most electron-deficient is the carbon atom bearing two nitro groups. On the other hand, reactions with nucleophiles involve the C^2 atom, as in β-nitrostyrene, for the corresponding intermediate anion is more stable than that formed via alternative nucleophilic attack at C^1.



Thus, joint analysis of the spectral data and results of quantum-chemical calculations allowed us to characterize molecules of β,β-dinitrostyrenes **IV**–**VI** as structures with nonequivalent nitro groups with respect to their interaction with the C=C bond; enhanced polarization and electrophilicity of the latter was assessed in comparison with model mononitrostyrene.

EXPERIMENTAL

The ^{1}H NMR spectra were measured on a Bruker AC-200 spectrometer (200 MHz) using chloroform-*d* as solvent and hexamethyldisiloxane as reference (internal or external); the chemical shifts were determined with an accuracy of ±0.5 Hz. The IR spectra were recorded on an InfraLYuM FT-02 spectrometer in chloroform (c = 40 mg ml^{-1}). The electronic absorption spectra were measured from solutions in chloroform on an SF-2000 spectrophotometer using quartz cells (cell path length 1 cm).

Quantum-chemical calculations of β,β-dinitrostyrenes **IV**–**VI** and model β-nitrostyrene (**I**) were performed using Gaussian 03w software package [19] in terms of the density functional theory [20] at the B3LYP/6-31+G* level of theory with account taken of diffuse and polarization functions.

Initial 1-nitro-2-phenylethene (**I**), 1-(*p*-chlorophenyl)-2-nitroethene (**II**), and 1-nitro-2-(*p*-tolyl)ethene (**III**) were prepared according to the procedures reported in [34–37]. 1,1-Dinitro-2-arylethenes **IV**–**VI** were synthesized by improved procedures [6, 7].

1,1-Dinitro-2-phenylethene (IV). A solution of 17 ml of dinitrogen tetraoxide in 14 ml of anhydrous carbon tetrachloride was added to a suspension of 4.00 g of 1-nitro-2-phenylethene (**I**) in 26 ml of anhydrous carbon tetrachloride, and the mixture was left to stand for 7 days at 16–18°C. Excess nitrating agent and the solvent were evaporated in the cold, the oily residue was treated with propan-2-ol, and the precipitate was filtered off. Yield 4.16 g (79%), light yellow crystals, mp 93–94°C (from anhydrous carbon tetrachloride); published data: mp 94–95°C (from CCl_4), yield 39% [6], 42.5% [7]. Found, %: C 49.60, 49.58; H 3.14, 3.12; N 14.40, 14.42. $C_8H_6N_2O_4$. Calculated, %: C 49.48; H 3.09; N 14.43.

2-(*p*-Chlorophenyl)-1,1-dinitroethene (V) was synthesized in a similar way from 1-(*p*-chlorophenyl)-2-nitroethene (**II**). Yield 2.24 g (49%), light yellow crystals, mp 70–71°C (from hexane); published data [7]: mp 69–70°C (from CCl_4), yield 39.5%. Found, %: C 42.12, 42.10; H 2.24, 2.23; N 12.22, 12.24. $C_8H_5ClN_2O_4$. Calculated, %: C 42.01; H 2.19; N 12.25.

1,1-Dinitro-2-(*p*-tolyl)ethene (VI) was synthesized in a similar way from 1-nitro-2-(*p*-tolyl)ethene (**III**). Yield 2.70 g (65%), light yellow crystals, mp 70–71°C (from hexane); published data [7]: mp 52–54°C (from CCl_4), yield 65.0%. Found, %: C 51.71, 51.70; H 4.05, 4.03; N 13.64, 13.67. $C_9H_8N_2O_4$. Calculated, %: C 51.92; H 3.85; N 13.46.

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