

AN ACCOUNT OF REGIOSELECTIVITY IN [2 + 3] CYCLOADDITION OF BENZONITRILE N-OXIDES WITH NITROETHENE BY PMO THEORY*

Andrzej BARAŃSKI^a and Gyula BÁNKI^b

^a Institute of Organic Chemistry and Technology,
Technical University, 31-155 Cracow, Poland

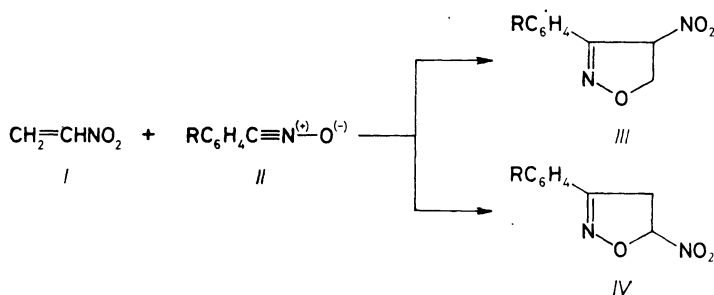
^b Department of Organic Chemistry,
Slovak Institute of Technology, 880 37 Bratislava, Czechoslovakia

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The application of PMO treatment to [2 + 3] cycloaddition of nitroethene to benzonitrile N-oxides is described. It was found that the reaction is under charge transfer control and PMO considerations based on MNDO calculations allow for the elucidation of the observed regioselectivity.

This contribution is intended as the continuation of our research dealing with an application of quantum-chemical methods to explain the reactivities¹⁻³ and regio-



In formulae II-IV: a, R = *p*-OCH₃ b, R = *p*-CH₃ c, R = *m*-CH₃ d, R = H
e, R = *p*-F f, R = *p*-Cl g, R = *m*-Cl h, R = *p, m*-Cl₂

SCHEME 1

* Part XXIX in the series: Synthesis and Properties of Azoles and their Derivatives; Part XXVIII: *Khim. Geterotsikl. Soed.* 1990, 1431. Some results of this work have already been presented at 1st International Symposium on Chemistry and Technology of Small-Tonage Products in Ufa (U.S.S.R.), July 17-19, 1987.

selectivities⁴⁻⁶ in organic reactions. In particular, in our earlier papers^{7,8} on the [2 + 3] cycloaddition reaction of nitroethene (*I*) to nitrile N-oxides (*II*), we remarked that the experimental results concerning the regioselectivity were in striking contrast to the expectations based upon the conventional electronic theories. Thus, instead of predicted 3-aryl-4-nitro-4,5-dihydro-1,2-oxazoles (*III*), within the experimental limits of detection (¹H NMR, TLC), 3-aryl-5-nitro-4,5-dihydro-1,2-oxazoles (*IV*) were obtained as the sole reaction products (Scheme 1). In order to rationalize this discrepancy the study of the reaction regioselectivity in terms of Perturbation Molecular Orbitals (PMO) theory⁹ was undertaken and the results are now reported.

RESULTS AND DISCUSSION

In accordance with PMO theory the regioselectivity of any chemical process can be predicted from the Salem-Klopman's equation⁹⁻¹¹, which represents the change of stabilization energy (ΔE) accompanying the interaction of the reactants. This change can be expressed by the sum of the three terms: the repulsion between the occupied orbitals (ΔE_1), the coulombic interactions between the reagents (ΔE_2) and the charge transfer interaction of the occupied orbitals of each molecule with the empty orbitals of the others (ΔE_3). The preferred transition state (TS) is that for which the larger ΔE is obtained.

In our study on regioselectivity the closed-shell repulsion was neglected due to Fleming's suggestion¹¹. Furthermore, considering the Fukui theorem¹², we limited the last term to frontier molecular orbitals (FMO) interactions only. Hence the equation can be re-written as follows:

$$\Delta E \sim \Delta E_2 + \Delta E_3 = - \sum_k \sum_l Q_k^S Q_l^R / \epsilon R_{kl} + 2 \left[\frac{(C_r^{\text{HO}} C_s^{\text{LU}} \beta_{rs} + C_{r'}^{\text{HO}} C_{s'}^{\text{LU}} \beta_{r's'})^2}{|E_s^{\text{LU}} - E_r^{\text{HO}}|} + \frac{(C_s^{\text{HO}} C_r^{\text{LU}} \beta_{rs} + C_{s'}^{\text{HO}} C_{r'}^{\text{LU}} \beta_{r's'})^2}{|E_r^{\text{LU}} - E_s^{\text{HO}}|} \right]. \quad (1)$$

In the expression (1) the marks R and S refer to nitroalkene *I* and N-oxides *II* respectively. Q_k^S and Q_l^R are the initial charges on the atoms *k* and *l*, whereas R_{kl} represents the distance between these atoms, and ϵ is the solvent dielectric constant. The C_r^{HO} , $C_{r'}^{\text{HO}}$, C_s^{HO} , $C_{s'}^{\text{HO}}$ are the HOMO eigenvectors of the atomic orbitals which have the bonding interaction in the TS; C_r^{LU} , $C_{r'}^{\text{LU}}$, C_s^{LU} , $C_{s'}^{\text{LU}}$ are the eigenvectors for the similar orbitals in LUMO; β_{rs} and $\beta_{r's'}$ are the resonance integrals of the bond developing between the reaction centers *r*...*s* and *r'*...*s'* in the transition state RS[‡]. The E_s and E_r are the energies of the interacting FMO's.

All these above values for nitroethene are available in the literature^{6,13,14} (Table I). For nitrile N-oxides, however, in the most cases they were not known. We have therefore evaluated the lacking values using the known algorithms and empirical

relationships. In particular, eigenvectors for FMO's and charge distributions were obtained from SCF MO calculations based on the MNDO approximation combined with full geometrical optimization by FPD procedure. As MNDO overestimated^{15,16} energies for FMO's the ones for HOMO levels were approximated by means of our own program¹⁷, which gives the energy for HOMO level in substituted benzenes with root mean square error no more than of 0.14 eV. The energy of LUMO levels can be obtained from electron transmission spectra¹⁸, reduction potentials¹⁹, charge transfer energies²⁰ or UV spectra²⁰⁻²². In this work they were evaluated from the empirical relation recommended by Houk et al.²¹ (Eq. 2), using transition energies $\Delta E_{\pi \rightarrow \pi^*}$ measured from electronic spectra and $(J_{ij} - 2K_{ij})$ values of 3.2 eV typical⁶ of aromatic nitrile N-oxides:

$$E_S^{LU} = E_S^{HO} + \Delta E_{\pi \rightarrow \pi^*} + (J_{ij} - 2K_{ij}) \quad (2)$$

The charge distributions on $C \equiv N \rightarrow O$ fragment, the eigenvalues and the selected eigenvectors of FMO's of N-oxides *IIa-IIIh* are collected in Table II.

The calculations of the coulombic interactions were performed on the assumption that the reactions are conducted in ether ($\epsilon = 4.34$ D)*. Moreover, the distances R_{kl}

TABLE I

Essential molecular properties of nitroethene: p_z coefficients of MNDO FMO's, energies of FMO's (in eV), the $\pi \rightarrow \pi^*$ energy (in eV), dipole moment μ (in D) and atomic charges (in e); for atomic positions see Fig. 1A-1F

HOMO			LUMO			$\Delta E_{\pi \rightarrow \pi^*}$	μ
C1	C2	$-E^{HO}$	C1	C2	$-E^{LU}$		
0.647	0.714	11.38 11.43 ^a	-0.615	-0.421	0.70 1.00 ^a	5.59	3.70
Total initial charges on atoms							
C1	C2	N7	H8	H9	H10	O11	O12
0.036	-0.092	0.470	0.112	0.066	0.082	-0.346	-0.332

^a MNDO data.

* $1 \text{ D} = 3.336 \cdot 10^{-30} \text{ C m.}$

TABLE II
Essential molecular properties of benzonitrile N-oxides *Ila–IIh*

Com- pound	R	Eigenvectors of the HOMO ^a			$-E^{\text{Hob}}$ eV	Eigenvectors of the LUMO ^a			$\Delta E_{\pi \rightarrow \pi^*}$ eV	$-E^{\text{Lub}}$ eV	Charge distribution on the atoms		
		C	N	O		C	N	O			C	N	O
<i>Ila</i>	<i>p</i> -CH ₃ O	0.330	0.236	-0.481	8.42 ^c (9.20)	0.187	-0.293	0.189	4.71	0.51 (0.81)	-0.136	0.271	-0.308
<i>IIb</i>	<i>p</i> -CH ₃	0.340	0.239	-0.493	8.72 (9.18)	0.196	-0.303	0.194	4.77	0.75 (0.71)	-0.134	0.271	-0.309
<i>IIc</i>	<i>m</i> -CH ₃	0.354	0.242	-0.511	8.91 (9.23)	0.205	-0.308	0.196	4.50	0.96 (0.64)	-0.133	0.270	-0.310
<i>IIId</i>	H	0.359	0.244	-0.516	8.96 ^c (9.24)	0.199	-0.313	0.208	4.77	1.00 (0.63)	-0.134	0.270	-0.309
<i>IIe</i>	<i>p</i> -F	0.343	0.237	-0.493	9.01 (9.36)	0.176	-0.286	0.187	4.70	1.11 (1.01)	-0.141	0.276	-0.303
<i>IIIf</i>	<i>p</i> -Cl	0.358	0.237	-0.506	9.06 (9.45)	0.178	-0.282	0.192	4.70	1.16 (1.03)	-0.144	0.280	-0.300
<i>IIg</i>	<i>m</i> -Cl	0.375	0.242	-0.527	9.28 (9.49)	0.186	-0.297	0.194	4.63	1.45 (0.96)	-0.143	0.280	-0.300
<i>IIh</i>	<i>m,p</i> -Cl ₂	0.369	0.234	-0.513	9.34 (9.65)	0.159	-0.278	0.186	4.64	1.50 (1.31)	-0.151	0.286	-0.292

^a The entries are the p_z coefficients; ^b in the parenthesis are given MNDO data; ^c data taken from ref.³³.

were assumed to be identical to ones in the regioisomeric TS's predicted by MNDO estimations for nitroethene [2 + 3] cycloaddition to formonitrile N-oxide (Table III). The structures of these TS's are shown schematically in Fig. 1. Their properties are discussed in details in other works^{1,2,3}.

From Eq. (1) it follows that if coulombic interactions contribute mainly to the stability of TS, one would be able to predict the preferred regioisomer from the values of ΔE_2 . Due to highly polarized structures of the reactants *I* and *II* we expected relatively large values of ΔE_2 . It was found, however, that for both regioisomeric TS's electrostatic interactions were relatively small. Moreover, they insignificantly favoured the formation of the unobserved regioisomers *III* (Table IV). Consequently, the coulombic interactions cannot be the origin of the regioselectivity in the studied reaction.

In Fig. 2 we depicted the perturbational diagram, performed on the basis on the eigenvalues taken from Tables I and II. As can be seen the energy gap between the HOMO of nitrile N-oxide and the LUMO of nitroethene is in each case smaller than that between the LUMO of nitrile N-oxide and the HOMO of nitroethene by more than 1.2 eV. This is the orbital arrangement typical of the normal electron demand for 1,3-dipolar cycloaddition²⁴ and indicates charge donation from 1,3-dipole to dipolarophile in TS. Therefore, the first fraction in the term ΔE_3 was neglected in evaluating the charge transfer energies. The resonance integrals required for calculations were taken from our previous paper⁶. There they were derived from the concerted TS's shown in Fig. 1 and are as follows: $\beta_{C-C} = 5.7$ and $\beta_{C-O} = 0.3$ eV for TS's leading to regioisomers *IV*, whereas for TS's leading to regioisomers *III* $\beta_{C-C} = 5.0$ and $\beta_{C-O} = 1.5$ eV.

TABLE III

Interatomic distances (Å) in transition states calculated (MNDO) for [2 + 3] cycloaddition of nitroethene to formonitrile N-oxide

Atoms	C1	C2	N7	H8	H9	H10	O11	O12
C3 ^a	2.70	1.83	3.62	2.22	2.20	3.30	4.32	4.10
N4 ^a	3.06	2.70	3.84	3.08	3.28	3.40	4.22	4.56
O5 ^a	3.31	3.40	3.93	3.80	4.13	3.35	3.96	4.84
C3 ^b	2.74	2.01	2.73	2.31	3.26	3.44	3.51	3.18
N4 ^b	2.80	2.70	3.54	3.16	3.17	3.29	4.03	4.24
O5 ^b	2.44	2.93	3.91	3.60	2.67	2.69	4.84	4.17

^a Fig. 1, A–C; ^b Fig. 1, D–F.

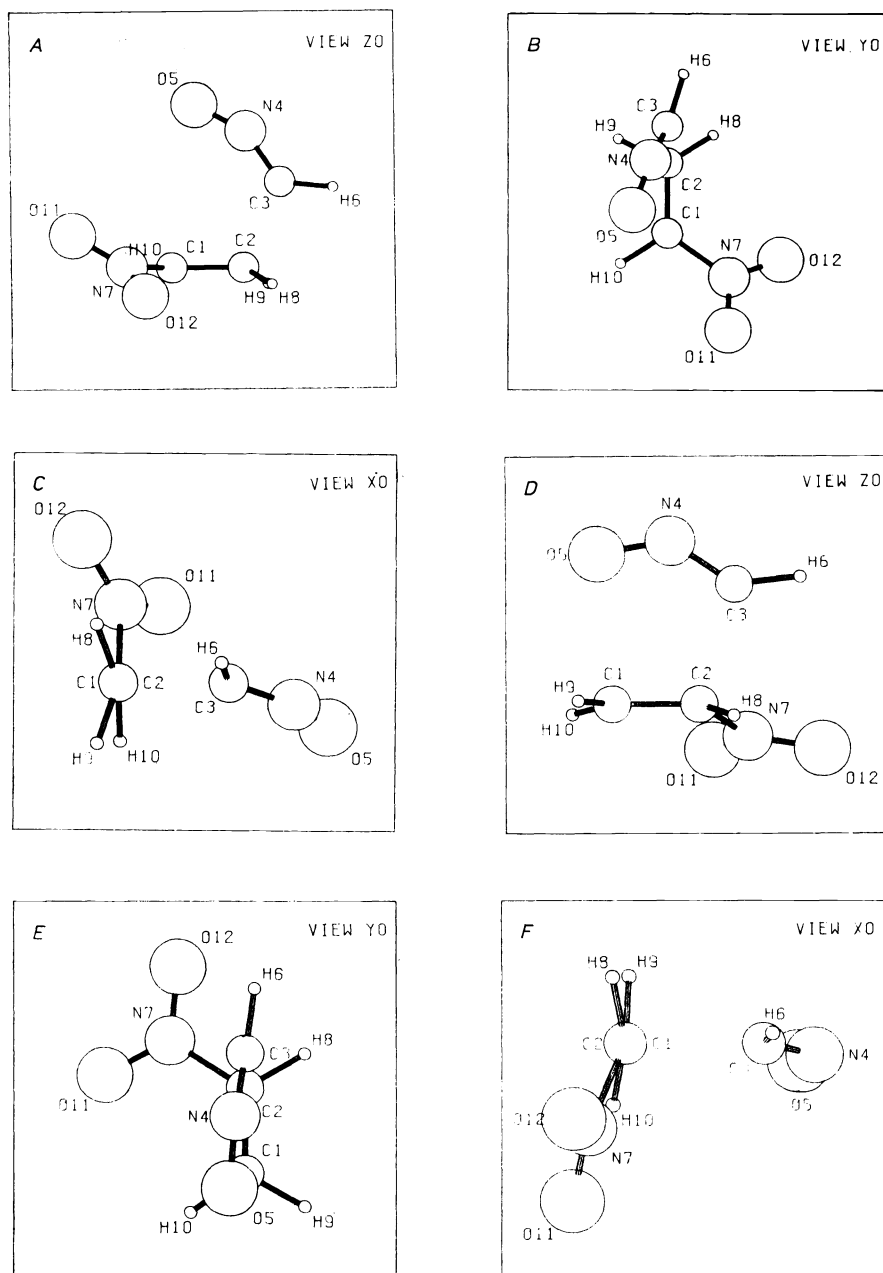


FIG. 1

The PLUTO views of the regioisomeric transition states calculated (MNDO) for [2 + 3] cycloaddition of formonitrile N-oxide to nitroethene (data for plots taken from ref.¹)

TABLE IV
Summarized results of coulombic, ΔE_2 , and charge transfer, ΔE_3 , stabilization energy (in kJ/mol) calculations

N-Oxide	ΔE_2^{III}	ΔE_2^{IV}	$\Delta E_2^{IV} - \Delta E_2^{III}$	$[IV]/[III]^a$	ΔE_3^{III}	ΔE_3^{IV}	$\Delta E_3^{IV} - \Delta E_3^{III}$	$[IV]/[III]^a$
<i>IIa</i>	2.58	1.51	-1.07	0.65	32.42	37.11	4.69	6.67
<i>IIb</i>	2.57	1.48	-1.09	0.65	33.00	37.90	4.90	7.25
<i>IIc</i>	2.58	1.48	-1.10	0.64	34.82	40.12	5.30	8.55
<i>IId</i>	2.59	1.49	-1.10	0.64	35.47	40.99	5.52	9.35
<i>IIe</i>	2.52	1.52	-1.00	0.67	32.04	37.02	4.98	7.52
<i>IIf</i>	2.58	1.51	-1.07	0.65	34.41	40.21	5.80	10.87
<i>IIg</i>	2.46	1.50	-0.96	0.68	36.63	42.96	6.33	13.70
<i>IIh</i>	2.38	1.53	-0.85	0.71	35.23	41.28	6.05	11.67

^a Calculated according to Eq. (3).

The calculations showed that the value of ΔE_3 obtained for TS leading to regioisomer *IV* was in each case considerably larger than for the one leading to regioisomer *III*. The ratios of the regioisomers estimated²⁵ according to the Eq. (3) on the basis of calculated values of ΔE_3 , are in reasonable agreement with the experimental data (Table IV).

$$[IV]/[III] = \exp\left(\frac{\Delta E_i^{IV} - \Delta E_i^{III}}{RT}\right) \quad (3)$$

Thus, the PMO theory nicely account for the regioselectivity in the [2 + 3] cycloaddition of nitroethene to aromatic nitrile N-oxides. It can be concluded that the reactions under study is governed by charge-transfer control and there is no evidence that the coulombic interactions have the dominant role in determining of its regioselectivity.

We would like to point out that physical properties of nitroisoxazolines *IVa*, *IVd*–*IVg* were presented in our previous papers^{7,8}. The nitroisoxazolines *IVb*, *IVc*, *IVh* are the new compounds. They were prepared from suitable benzonitrile N-oxides and nitroethene and their structure was established on the basis of the elemental analysis, IR and ¹H NMR spectral data. Consequently, the presence of the bands in the IR spectra in the frequency range of 825–790, 1 370–1 360 and 1 575–1 570, 1 615–1 590, 1 065–1 060, 860–840 cm⁻¹ (see Experimental) are

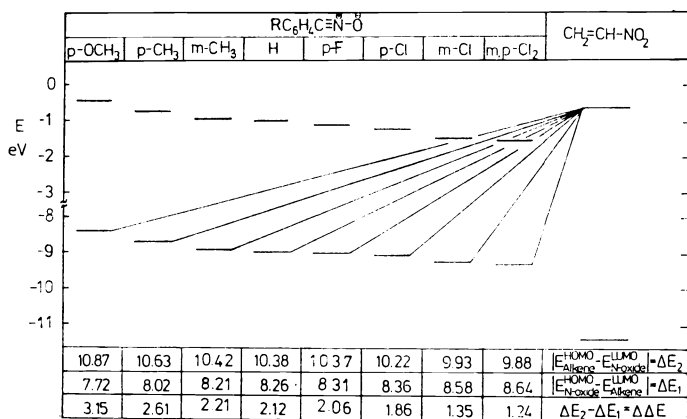


FIG. 2

Diagram of FMO interaction of benzonitrile N-oxides *Ila*–*Ilh* with nitroethene

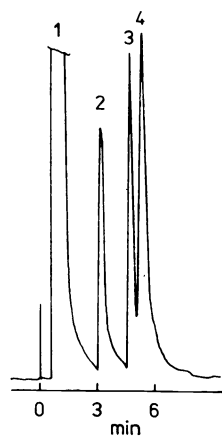


FIG. 3

The chromatogram of post-reaction mass of 3-(*m*-methylphenyl)-5-nitro-4,5-dihydro-1,2-oxazole (*IVc*) with diethylamine: 1 solvent, 2 N-nitrosodiethylamine, 3 N,N-diethylacetamide, 4 *m*-methylbenzonitrile

indicative of the existence of aromatic rings²⁶, unconjugated nitro group²⁷, >C=N—bond^{28} , >C=N—O—C fragment²⁸ and 4,5-dihydro-1,2-oxazole ring²⁹, respectively. The ^1H NMR spectra confirmed the presence of the aromatic protons, methyl groups connected with the phenyl ring as well as 3,5-disubstituted 4,5-dihydro-1,2-oxazole ring protons⁸ which form the ABX-type system. Additional confirmation of the regiochemistry was obtained from the results of the chemical transformation of 3-(*m*-methylphenyl)-5-nitro-4,5-dihydro-1,2-oxazole (*IVc*). Thus the treatment of this compound with the excess of diethylamine resulted in characteristic^{8,30} of 5-nitro-4,5-dihydro-1,2-oxazoles ring opening to give N-nitrosodiethylamine (*V*), N,N-diethylacetamide (*VI*) and *m*-methylbenzotrile (*VII*) (Fig. 3).

EXPERIMENTAL

The MO calculations presented in this work were carried out on CYBER-72 (Cyfronet, Cracow) and M-3040 (SVŠT, Bratislava) computers.

Melting points (uncorrected) were determined on a Boetius plate. The ^1H NMR spectra were recorded on Tesla BS-487C spectrometer in CD_3NO_2 solutions using TMS ($\delta = 0.0$ ppm) as internal standard. IR absorption spectra were taken on UR-20 (C. Zeiss) spectrophotometer using standard KBr technique. The composition of products and their purity were checked by means of thin-layer chromatography (TLC). Silica gel plates (Silufol UV 254) and the mixture of cyclohexane and ethyl acetate (at various ratios) were used. Gas chromatographic (GC) analyses were carried out on Hewlett-Packard instrument equipped with an FI detector and 1.5 m glass column containing UCW-987 on chromosorb P. Benzotrile N-oxides *IIf*, *IIfc* and *IIfh* were prepared from suitable hydroxamic acid chlorides as described previously³¹. Nitroethene (*I*) was prepared from nitromethane and formaldehyde according to the literature method³².

Cycloaddition of Benzotrile N-Oxides *IIf*, *IIfc*, *IIfh* with Nitroethene *I*. General Procedure

To a vigorously stirred and ice cooled solution of suitable nitrile N-oxide (0.01 mol) in diethyl ether (50 ml) nitroethene (1.46 g, 0.02 mol) was added and reaction mixture was kept at room temperature for 24 h. The solvent together with excess of alkene was removed under vacuum. The solid residue was tested by means of TLC and ^1H NMR spectroscopy and then was purified by crystallization from suitable solvent.

Thus, from *p*-methylbenzotrile N-oxide (*IIf*) and nitroethene, 3-(*p*-methylphenyl)-5-nitro-4,5-dihydro-1,2-oxazole *IVb* (1.71 g, 83%), m.p. 104–106°C was obtained. For $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_3$ (206.2) calculated: 58.25% C, 4.85% H, 13.59% N; found: 58.10% C, 4.98% H, 13.34% N. IR spectrum, cm^{-1} : 825, 1360, 1575, 1615, 1060, 840. ^1H NMR spectrum: 2.43 s, 3 H; 3.98 dd, 1 H ($J = 18.9, J = 4.3$); 4.31 dd, 1 H ($J = 18.9, J = 7.3$); 6.34 dd, 1 H ($J = 7.3, J = 4.3$); 7.31 d, 2 H ($J = 9.0$); 7.66 d, 2 H ($J = 9.0$).

Similarly, from *m*-methylbenzotrile N-oxide (*IIfc*) and nitroethene 3-(*m*-methylphenyl)-5-nitro-4,5-dihydro-1,2-oxazole *IVc* (1.76 g, 85%), m.p. 76–79°C (light petroleum) was obtained. For $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_3$ (206.2) calculated: 58.25% C, 4.85% H, 13.59% N; found: 58.52% C, 4.90% H, 13.37% N. IR spectrum, cm^{-1} : 790, 1360, 1570, 1610, 1065, 845. ^1H NMR spectrum: 2.42 s, 3 H; 3.96 dd, 1 H ($J = 19.0, J = 4.3$); 4.30 dd, 1 H ($J = 19.0, J = 7.1$); 6.35 dd, 1 H ($J = 4.3, J = 7.1$); 8.0–7.4 m, 4 H.

Analogously, from *m,p*-dichlorobenzonitrile N-oxide (*IIh*) and nitroethene 3-(*m,p*-dichlorophenyl)-5-nitro-4,5-dihydro-1,2-oxazole *IVh* (2.20 g, 84%), m.p. 90–92°C (ethanol) was obtained. For $C_9H_6Cl_3N_2O_3$ (261.5) calculated: 41.38% C, 2.30% H, 10.73% N; found: 41.64% C, 2.52% H, 10.86% N. IR spectrum, cm^{-1} : 820, 1 370, 1 570, 1 590, 1 060, 860. 1H NMR spectrum: 3.95 dd, 1 H ($J = 19.0, J = 3.8$); 4.29 dd, 1 H ($J = 19.0, J = 7.0$); 6.46 dd, 1 H ($J = 3.8, J = 7.0$); 7.88–7.63 m, 3 H.

Reaction of 3-(*m*-Methylphenyl)-5-nitro-4,5-dihydro-1,2-oxazole (*IVc*) with Diethylamine

To a solution of nitroisoxazoline *IVc* (100 mg, 0.5 mmol) in chloroform (ca 1.0 ml) diethylamine was added at room temperature. The mixture was shaken for 20 min and then tested by means of GC. Analysis was performed under the following conditions: injector temperature 150°C, column temperature 130°C, carrier gas helium. The presence of N-nitrosodiethylamine (*V*), N,N-diethylacetamide (*VI*) and *m*-methylbenzonitrile (*VII*) in the post-reaction mixture was confirmed by comparing the retention times of the obtained compounds with those of the standard samples. A typical chromatogram is shown in Fig. 3.

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