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Solvatochromism of Heteroaromatic Compounds: XIV.[1] 5-Amino-1-methyl-4-nitropyrazole and Its Analogs

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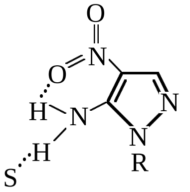
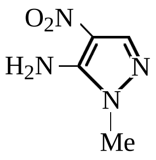
Abstract—The solvatochromism of H complexes of 5-amino-1-methyl-4-nitropyrazole and 2-nitroaniline derivatives in aprotic protophilic media was described on a quantitative level with the aid of Kamlet–Taft empirical parameters. Specific solvation affects only one of the two long-wave bands, namely that corresponding to an electronic transition involving orbital electron density transfer from the H-bound nitrogen atom. When such transfer does not occur, which is typical of the second transition, specific solvatochromic effect is either weak or absent.

Electronic absorption spectra of *ortho*-aminonitropyrazoles, in particular of 4-amino-1-methyl-5-nitropyrazole, are very similar to the spectrum of 2-nitroaniline. On the basis of this analogy Perevalov *et al.* [2, 3] assigned the absorption bands and established the nature of the coorresponding electronic transitions with a sufficient reliability. The data of IR spectroscopy indicated formation of intramolecular hydrogen bond in the ground state of *ortho*-aminonitropyrazoles. The H bond turned out to be weaker than the intramolecular hydrogen bond in 2-nitroaniline [2]. The difference was explained by reduction of bond angles in going from a six-membered ring to five-membered and increased basicity of the amino group in pyrazoles. According to [2, 3], the long-wave $\pi \rightarrow \pi^*$-transition involves redistribution of the orbital electron density from the amino to nitro group. Therefore, the strength of the intramolecular hydrogen bond should change in going to the Franck–Condon excited state. A question arises so as to how does vertical transition to the first excited state affect the intramolecular hydrogen bond formed by *ortho*-aminonitropyrazoles with a protophilic solvent S.

The second $\pi \rightarrow \pi^*$ transition does not involve the amino group. It occurs from that π MO which contributes most to the total charge on atoms of the heteroring (the orbital electron density distribution, calculated by the MNDO method, was given in [3]). Taking into account that both long-wave absorption bands of *ortho*-aminonitropyrazoles are well-resolved and fairly intense, we have analyzed spectral effects of specific solvation on $\pi \rightarrow \pi^*$ transitions involving different intramolecular charge distribution patterns, using 5-amino-1-methyl-4-nitropyrazole (**I**) as example. The amino and nitro groups in molecule **I** are separated by a bond having a higher order than the corresponding bond in 2-nitroaniline (**II**). Therefore, their solvatochromic parameters can be compared directly.

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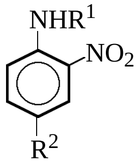
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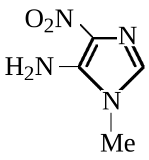
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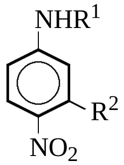
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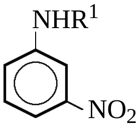
XV, XVI

II–V, **IX**, **XIII**, **XV**, R^1 = H; **VI**, R^1 = NH_2; **VIII**, **X**, R^1 = Me; **XI**, **XIV**, **XVI**, R^1 = Et; **XII**, R^1 = *i*-Pr; **II**, **VIII–XII**, R^2 = H; **III**, **XIII**, **XIV**, R^2 = H; **IV**, R^2 = OMe; **V**, **VI**, R^2 = NO_2.

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[1] For communication XIII, see [1].

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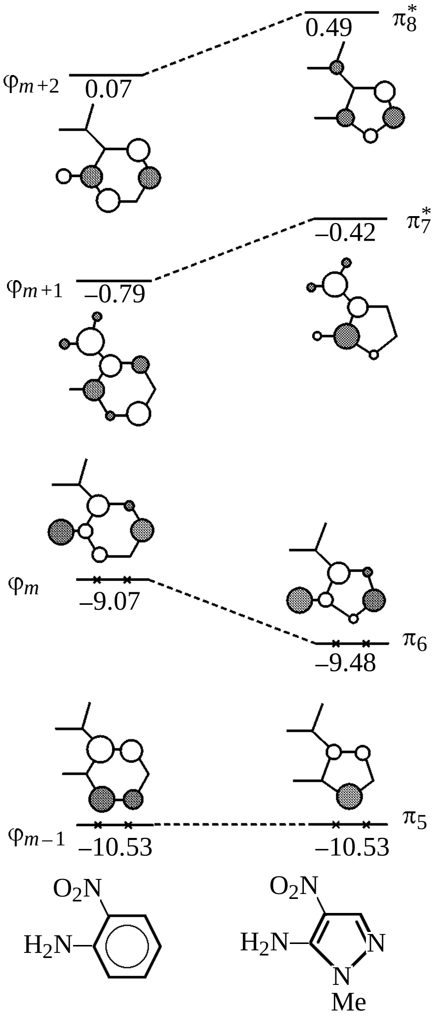


Orbital correlation diagram for 2-nitroaniline and 5-amino-1-methyl-4-nitropyrazole, according to AM1 calculations. The orbital energies are given in eV.

The figure shows the orbital correlation diagram for compounds **I** and **II**, which was plotted on the basis of AM1(CI) calculations. The parameters of two low-energy $\pi \rightarrow \pi^*$ transitions, calculated by the same method, are given in Table 1. Analysis of these data shows that the assignment of $\pi \rightarrow \pi^*$ transitions made in [2, 3] in terms of π-electron approximation is confirmed by the results of a more accurate procedure. According to the latter, the $\pi_6 \rightarrow \pi_7^*$ transition in the UV spectra of *ortho*-aminonitropyrazoles and *ortho*-nitroanilines results in decrease of the orbital electron density not only on the amino nitrogen atom, but also on the N^2 atom of the heteroring, as well as in some redistribution of the orbital electron density over carbon atoms of the six-membered ring. The next $\pi \rightarrow \pi^*$ transition, in keeping with the AM1(CI) data, is not one-electron. The excited state thus formed is the result of interaction of two singly excited configurations, only one of which corresponds to a locally excited state with intramolecular charge transfer to the nitro group (see figure). Nevertheless, the second $\pi \rightarrow \pi^*$ transition can also be sufficiently sensitive to nonspecific solvation, for the predominant configuration is Ψ_{m-1}^{m+1} and the electron density distributions at π_5 MO and π_7^* MO are essentially different. In order to substantiate this assumption on an empirical level, we examined nonspecific solvatochromic effects for 2-nitro-4-methylaniline (**III**), 2-nitro-4-methoxyaniline (**IV**), 2,4-dinitroaniline (**V**), 2,4-dinitrophenylhydrazine (**VI**), and 5-amino-1-methyl-4-nitroimidazole (**VII**). Solvatochromic parameters of compounds **I**–**III** and **V**–**VII** (as regards their long-wave absorption bands) are given in Tables 2 and 3. With the goal of examining effects of both nonspecific and specific solvatation we used aprotic inert and protophilic solvents (containing no aromatic fragments). Multiple linear regression analysis with the aid of Kamlet–Taft solvatochromic parameters [4, 5] was applied.

Table 1. Parameters of long-wave $\pi \rightarrow \pi^*$ transitions in compounds **I** and **II**, according to AM1(CI) semi-empirical calculations

Comp. no.	Transition	ν, cm^{-1}	Transition moment (CNDO/S)	Configurational composition[a]
I	$\pi_6 \rightarrow \pi_7^*$	31 600	0.45	$0.61\Psi_m^{m+1}$
	$\pi \rightarrow \pi^*$	33 100	0.30	$0.45\Psi_{m-1}^{m+1}$, $0.37\Psi_m^{m+2}$
II	$\pi_6 \rightarrow \pi_7^*$	28 300	0.54	$0.60\Psi_m^{m+1}$
	$\pi \rightarrow \pi^*$	32 600	0.45	$0.37\Psi_{m-1}^{m+1}$, $0.54\Psi_m^{m+2}$

[a] The transition $\varphi_i^2 \rightarrow \varphi_j^0$ corresponds to the configuration Ψ_i^j.

$$\nu_{max} = \nu_0 + b\beta + s\pi^* + e\xi.$$

Here, $\nu_0 = \nu_{max}$ at $\beta = \pi^* = \xi = 0$; β is a solvent parameter characterizing its proton-acceptor power in H complex with the solute; π^* is a parameter characterizing the ability of solvent to stabilize dipolar molecules or ions; and ξ is an approximate covalent constituent of the coordination bond. The regression coefficients and free terms of the above equation, which is valid for both initial compounds and H complexes derived therefrom, are given in Table 4.

The crucial role of the Ψ_{m-1}^{m+1} configuration in the second electronically excited state of pyrazole (**I**) is confirmed by analysis of the low-energy part of its photoelectron spectrum reported in [3]. Let us assume that both long-wave $\pi \rightarrow \pi^*$ transitions in **I** are one-electron ($\nu^{(1)}$ corresponds to $\varphi_m \rightarrow \varphi_{m+1}$, and $\nu^{(2)}$, to $\varphi_{m-1} \rightarrow \varphi_{m+1}$). The difference in their energies is equal to the difference in the energies of ionization from φ_m and φ_{m-1} π MOs. According to the first two

Table 2. Solvatochromic parameters of compounds **I**–**III** in aprotic protophilic solvents

Solvent	Kamlet–Taft parameters[a]			**I**		**II**		**III**	
	β	π^*	ξ	ν^1_{max}, cm^{-1}	ν^2_{max}, cm^{-1}	ν^1_{max}, cm^{-1}	ν^2_{max}, cm^{-1}	ν^1_{max}, cm^{-1}	ν^2_{max}, cm^{-1}
Triethylamine	0.71	0.14	1.00	30350	–	25650[b]	–	–	–
Dibutyl ether	0.46	0.24	0.20	30750	38100	25650	36650	24800[c]	36200
Diethyl ether	0.47	0.27	0.20	30600	38100	25650[b]	36650[b]	24700	36250
Diisopropyl ether	0.49	0.27	0.20	30650	38250	25550	36650	24700	36200
Dioxane	0.37	0.55	0.20	30000	37350	25250[b]	36250[b]	24400[c]	35850
Ethyl acetate	0.45	0.55	0.00	30050	–	25200[d]	36350[d]	24350[c]	35900
THF	0.55	0.58	0.00	29900	37350	25000[c]	36200	24200[c]	35850
Triethyl phosphate	0.77	0.72	–0.20	–	–	24650[b]	–	23850[b]	–
Acetonitrile	0.31	0.75	0.10	29650	36900	25000[b,e]	36100[b]	24150[e]	35650
Propylene carbonate	0.40	0.83	0.00	29350	36650	24650	35950	23800	35550
Nitromethane	0.25	0.85	0.00	29600	–	24900	–	23950	–
HMPA	1.05	0.87	–0.20	29050	36750	23950	35750	23200	35400
DMF	0.69	0.88	0.00	29000	36600	24350[b]	–	23550[b]	–
1-Methyl-2-pyrrolidone	0.77	0.92	0.00	28900	36550	24250[c]	35750	23450[c]	35400
DMSO	0.76	1.00	0.00	28600	36250	24100[b]	35700[c]	23350[c]	35250

[a] The parameters were taken from [4, 5]. [b] Data of [6–8]. [c] Average value of ν_{max} from [7, 8] and the present work. [d] Given are values for methyl acetate (β = 0.42, π^* = 0.60) from [6]; in ethyl acetate, for ν^1_{max} = 25 300 cm^{-1} [7]. [e] The ν^1_{max} values for compounds **II** and **III**, measured in acetone (β = 0.48, π^* = 0.71), are 24 850 and 24 050 cm^{-1}, respectively.

Table 3. Solvatochromism of the long-wave absorption bands of compounds **V**–**VII** in aprotic protophilic solvents

Solvent	Kamlet–Taft parameters[a]			ν^1_{max}, cm^{-1}		
	β	π^*	ξ	**V**[b]	**VI**[b]	**VII**
Triethylamine	0.71	0.14	1.00	30450	29000[c]	[d]
Dibutyl ether	0.46	0.24	0.20	30750	29100[c]	~29500[d]
Diethyl ether	0.47	0.27	0.20	30700	29250[c]	~29500[d]
Diisopropyl ether	0.49	0.27	0.20	30850	29350[c]	[d]
Butyl acetate	0.45	0.50	0.00	30050	28900	28650
1,2-Dimethoxyethane	0.41	0.53	0.20	–	28750	28450
Dioxane	0.37	0.55	0.20	30000	28750	28500
Ethyl acetate	0.45	0.55	0.00	29900	28600	28650
THF	0.55	0.58	0.00	29750	28500	28350
Ethyl trichloroacetate	0.25	0.61	0.00	30200	28600	–
Ethyl chloroacetate	0.35	0.70	0.00	29800	28150	28250
Acetonitrile	0.31	0.75	0.10	29650[e]	28050	27950
Propylene carbonate	0.40	0.83	0.00	29300	27850	27800
Tetramethylurea	0.80	0.83	0.00	28800	27550	27700
HMPA	1.05	0.87	–0.20	28550	27450	27650
Butyrolactone	0.49	0.87	0.00	29100	–	27750
DMF	0.69	0.88	0.00	28900	27450	27550
Dimethylacetamide	0.76	0.88	0.00	28700	27400	27550
1-Methyl-2-pyrrolidone	0.77	0.92	0.00	28700	27250	27550
DMSO	0.76	1.00	0.00	28450	27050	27250

[a] The parameters were taken from [4, 5]. [b] The long-wave absorption band is split into two components due to the presence of two nitro groups; the data are given for the short-wave component; the second component appears as a shoulder at ν 24 000–26 000 cm^{-1}.
[c] The observed absorption maximum is a superposition of bands belonging to the monomeric species and self-associates, which exist in a dynamic equilibrium; the given values were not taken into account while calculating solvatochromic parameters. [d] Measurement of ν^1_{max} was difficult because of the very poor solubility; the approximate values were not used in the calculation of coefficients for the solvatochromic equation. [e] In acetone (β = 0.48, π^* = 0.71), ν^1_{max} = 29 700 cm^{-1}.

Table 4. Solvatochromic parameters of *ortho*-nitro compounds **I**–**VII** in aprotic protophilic solvents and dipole moments of their H complexes with dioxane

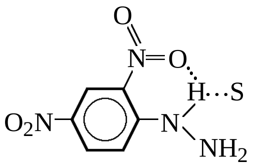
Comp. no.	μ_g,[a] D	ν_0, cm^{-1}	–*b*, cm^{-1}	–*s*, cm^{-1}	–*e*, cm^{-1}	*R*	*s*	*n*
I	6.06	31820±90	750±100	2550±110	610±120	0.987	80	14
		38780±60	–	2480±90	–	0.994	80	11
II	4.62	26590±50	1040±80	1710±60	–	0.987	60	17
	4.68[b], 4.36[b]	37080±50	260±80	1210±70	–	0.982	50	11
III	4.61	25580±50	850±70	1620±60	–	0.988	50	15
		36600±30	140±50	1210±40	–	0.992	30	11
IV[c]		24140±110	500±260	1720±170	–	0.982	70	8
V	6.53[b], 6.48[b]	32080±80	1220±110	2710±120	380±120	0.988	80	20
VI	6.90	30710±70	410±90	3360±130	–	0.991	60	15
VII		30220±90	320±100	2720±120	720±190	0.985	60	15

[a] In dioxane at 25°C. [b] Published data [9–12]. [c] Experimental data from [7, 8].

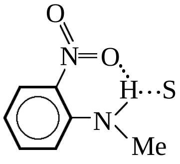
ionization potentials of pyrazole **I**, given in [3], this difference is about ~7200 cm^{-1}; in keeping with the UV spectral data, the difference $\nu_0^{(2)} - \nu_0^{(1)}$ is equal to 6960 cm^{-1} (Table 4).

Taking into account that spectral shifts are additive, the nonspecific solvatochromic effect for a particular compound is determined by the coefficient *s* ($\Delta\nu = s\pi^*$). As follows from Table 4, the values of *s* for two low-energy electronic transitions are almost similar. This is explained by the fact that in both cases orbital electron density transfer to the nitro group occurs mainly from the nitrogen atom either of the amino group or of the pyrazole ring (see figure and Table 1). The first and second long-wave absorption bands of 2-nitroanilines show different sensitivities to nonspecific solvation (Table 4), since the second electronic transition involves charge transfer from the ring containing no heteroatoms. Thus, any general relations holding in the effect of nonspecific solvation on absorption spectrum in the series of 4-nitropyrazoles and 2-nitroanilines may be found only for those transitions which involve considerable change of electron density on the heteroatom. In particular, we observed the expected increase of nonspecific solvatochromic effect (which is expressed by the regression coefficient *s*) for the long-wave absorption band with increasing dipole moment of the H complexes with dioxane in the ground state (Table 4). Analogous pattern was observed previously for isomeric nitropyrazoles [13] and some other compounds [14].

The spetcific solvatochromic effect is determined by the coefficient *b*. Its absolute value for the first absorption band of compound **I** is considerably larger than for the second band (Table 4). The negative sign of *b* means that the formation of H complex with the solvent is accompanied by a red shift of the absorption bands. Hence the intermolecular hydrogen bond becomes stronger in going to the Franck–Condon excited state. The specific solvatochromic effect ($\Delta\nu_H = b\beta$), as well as nonspecific, depends on the structure of proton donor. For example, it ranges from ~0.5 to ~3.5 kcal/mol for the first absorption band of compounds **I**–**VII** in DMSO (β = 0.76) (Table 4). Compounds **VI** and **VII** are characterized by minimal $\Delta\nu_H$ values. The structure of 2,4-dinitrophenylhydrazine (**VI**) assumes formation of a bifurcation (three-center) hydrogen bond with a protophilic solvent S.



VI



VIII

However, this assumption disagrees with the results of treatment of the experimental data reported in [15] on solvatochromic properties of *N*-methyl-2-nitroaniline (**VIII**), which is also capable for analogous interactions (in addition, we obtained $\nu^1_{\max}$ in dibutyl and diethyl ethers: 24 150 and 24 100 cm^{-1}, respectively). In aprotic protophilic solvents, the following equation is valid:

$$\nu^1_{\max} = (24640 \pm 70) - (140 \pm 200)\beta - (1610 \pm 120)\pi^*;$$

$$R = 0.987,\ s = 50,\ n = 9.$$

This equation suggests that the spectral shifts of the long-wave absorption band of compound **VIII** are determined mainly by nonspecific solvation (cf. [8]).

Table 5. Solvatochromic parameters of *para*- and *meta*-nitroanilines[a] in aprotic protophilic solvents and dipole moments of their 1:1 H complexes with dioxane

Comp. no.	μ_g,[b] D	ν_0, cm^{-1}	$-b$, cm^{-1}	$-s$, cm^{-1}	*R*	*s*	*n*
IX	6.80	30890 ± 80	2480 ± 130	3330 ± 90	0.988	110	27
X	7.12	29060 ± 70	890 ± 120	3350 ± 90	0.993	70	18
XI		28990 ± 70	810 ± 120	3490 ± 90	0.993	80	18
XII		28760 ± 90	640 ± 150	3490 ± 110	0.988	100	18
XIII		30890 ± 80	2470 ± 160	3050 ± 120	0.993	80	17
XIV		29040 ± 70	990 ± 130	3100 ± 110	0.991	80	17
XV	5.24	29160 ± 70	3150 ± 110	1720 ± 90	0.991	80	19
XVI	5.51	27300 ± 40	1650 ± 70	2110 ± 50	0.995	50	19

[a] The experimental data were taken from [6,15–23]. [b] Published data for dioxane [24].

Therefore, the most probable hypothesis is that the formation of H complex through the terminal amino group of **VI** leads to some variation of the state of the intramolecular hydrogen bond. The formation of an intermolecular H complex between 2,4-dinitrophenylhydrazine and protophilic medium is supported by the very strong effect of the chemical nature of the solvent on the dipole moment of **VI** in the ground state (μ_g 5.59 D in benzene and 6.90 D in dioxane at 25°C).

Before considering specific solvatochromic effects in the series of *ortho*-nitro derivatives under study, it seems reasonable to give some information on *meta*- and *para*-nitroanilines, whose solvatochromic properties were studied in detail in [6, 15–23]. Table 5 contains the results of analysis of the average ν_{max} values, measured in aprotic protophilic media, with the aid of the Kamlet–Taft parameters. Let us emphasize once more that protophilic solvents having an aromatic fragment were not included. The data in Table 5 lead us to the following conclusions. First, the specific solvatochromic effect arising from formation of intermolecular hydrogen bond for *meta*- and *para*-nitroanilines is not always additive (cf. **IX** and **X**–**XII**, **XIII** and **XIV**, **XV** and **XVI**, and data of [8, 18]).[2] Second, the regression coefficient *b* does not remain constant in the series of analogous 3- and 4-isomers (Table 5). Different *b* values are also obtained for 4-isomers differing by branching of the alkyl group on the amino nitrogen atom. This means that such variations of the H-donor structure change the relation between the energies of the corresponding H complexes with the solvent in the ground and Franck–Condon excited states. The specific solvatochromic effect for compounds in which the amino group is located *ortho* with respect to the nitro group (Table 4) strongly depends on the structure of the ring, and in some cases it is comparable with that found for *N*-alkyl-4-(or 3-)nitroanilines. Probable reasons are both variation of the electronic effect of the nitro group (cf. 3- and 4-nitroanilines) and formation of intramolecular hydrogen bond. The two reasons are likely to be closely interrelated, for change of the substituent and ring structure leads to considerable variations in the specific solvatochromic effect in the series of *ortho* isomers (Table 4). In particular, the coefficient *b* for 2-nitroaniline is larger than that for 5-amino-1-methyl-4-nitropyrazole whose intramolecular hydrogen bond in the ground state is less stronger [2].

The weakening of the effect of specific solvation on the solvatochromism of *orto*-nitro compounds in the series **V** > **II** > **III** > **I** > **IV** > **VI** > **VII** is explained primarily by reduced degree of orbital electron density transfer from the amino group upon excitation. This directly follows from the dependence of $\Delta\nu_H$ on the *para* substituent in 2-nitroanilines (NO_2 > H > Me > OMe) and from the considerably lower specific solvatochromic effect for the second absorption band of compounds **I**–**III** (as compared to the first one; Table 4). As we already noted, the second $\pi \to \pi^*$ transition does not appreciably change of the orbital electron density on the amino nitrogen atom. The above stated may be regarded as evidence of the applicability of the concept of electrostatic nature of hydrogen bonding to nonequilibrial excited charge-transfer states of unsym-metrical complexes with a normal intramolecular hydrogen bond. At least, there is no need of invoking the concept of three-center four-electron interaction (3*c*4*e*) [25] for qualitative analysis of the revealed relations.

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[2] The nonadditivity is masked when all kinds of aprotic solvents are analyzed jointly [8].

EXPERIMENTAL

The electronic absorption spectra were recorded on a Specord UV-Vis spectrophotometer at 22–25°C. Quantum-chemical calculations of the orbital structure and energies of $\pi \rightarrow \pi^*$ transitions for compounds **I** and **II** were performed in the AM1 approximation [26] with allowance for configurational interactions (200 configurations arising from electron excitation from six occupied molecular orbitals to six vacant MOs were considered).

Compound **I** was synthesized by the procedure reported in [27]. Its melting point was 264–266°C, which is consistent with the data for the same compound prepared as described in [28]. The product was purified by recrystallization first from methanol and then from hot water.

5-Amino-1-methyl-4-nitroimidazole (VII). Trimethylhydrazinium iodide, 5.45 g, was slowly added while stirring to a solution of 3.15 g of 1-methyl-4-nitroimidazole in 40 ml of anhydrous DMSO. The mixture was stirred at 25°C until it became homogeneous, and 2.92 g of anhydrous sodium methoxide was added. After 5–7 min, the mixture acquired an intense red color. It was stirred for 10 h, poured onto ice, and acidified to pH 3.0 with 10% hydrochloric acid. The precipitate of imidazole **VII** was filtered off, and the filtrate was extracted with three portions of ethyl acetate. The extracts were combined, dried over $MgSO_4$, and evaporated under reduced pressure. The residue was combined with the precipitate and recrystallized first from DMF and then from hot water. Yield 1.86 g (56%), mp 295–297°C; published data [29]: mp 297°C. The purity of the product was checked by physical methods.

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