Ring-Chain Tautomerism of 3,5-Disubstituted 5,6,7,8-Tetrahydro-3H-[1,2,4]oxadiazolo[4,3-*c*]pyrimidine, a Novel Heterocyclic Ring System

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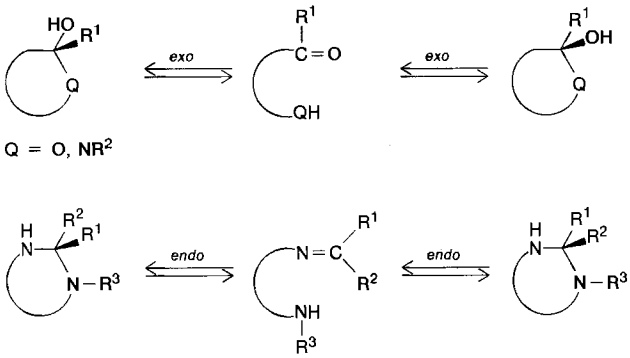
The reaction of 3-aminopropionamide oxime (**7**) with two equiv. of benzaldehyde or of a substituted benzaldehyde gives *cis*-3,5-diaryl-5,6,7,8-tetrahydro-3*H*-[1,2,4]oxadiazolo[4,3-*c*]-pyrimidines (*cis*-**11a-c,e**). According to ^{1}H-, ^{13}C-, and ^{15}N-NMR studies these compounds form in solution a novel triple tautomeric equilibrium comprising *cis*- and *trans*-**11a–c, e** and 3-[2-(benzylidineamino)ethyl]-5-aryl-4,5-dihydro-1,2,4-oxadiazoles (**10a–c, e**). However, the solid obtained from **7** and two equiv. of cinnamaldehyde proved to be an imine (**10g**), which again formed in solution a similar triple tautomeric system analogously to the mutarotation of sugars. The structure of **11a** and **10g** was confirmed by X-ray crystallography.

It is well known that in reversible intramolecular addition reactions cyclic stereoisomers may equilibrate in solution via open-chain intermediates. Mutarotation of sugars is a thoroughly studied example[1] but similar ring-chain tautomeric systems have been observed with other ring systems, too, e.g. with nitrogen heterocycles[2]. These triple tautomeric equilibria generally correspond to the *exo* type[3] of Scheme 1.

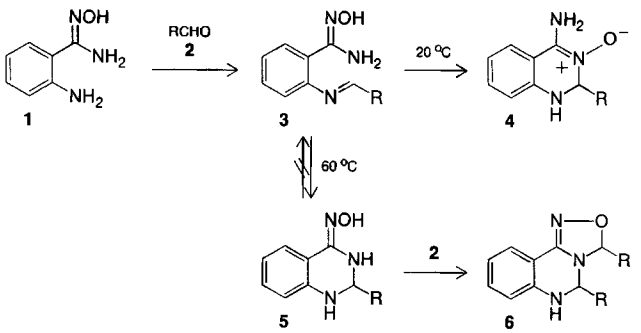
Scheme 1



Our studies on ring-chain tautomerism and ring transformations of pyrimidines[4] led to the discovery of [1,2,4]oxadiazolo[4,3-*c*]pyrimidines, a new heterocyclic ring system, which forms in solution a tautomeric system corresponding to the *endo*[3] type in Scheme 1. To the best of our knowledge there has been no example reported so far for such a triple ring-chain tautomeric system involving amine addition to a C=N bond.

Earlier we have described that in the reaction of 2-aminobenzamide oxime (**1**) with aldehydes (**2**) at room temperature 4-aminoquinazoline 3-oxides (**4**) are formed which isomerize above 60 °C to 4-quinazoline oximes (**5**)[4b]. Whith a second equiv. of the aldehyde, **5** is transformed into the oxadiazoloquinazoline **6**[4b,5]. No tautomeric equilibria have been detected in these reactions (Scheme 2).

Scheme 2



Gonçalves and co-workers found[6] that in the reaction of the aliphatic analogue of **1**, i.e. 3-aminopropionamide oxime (**7**), with one equiv. of aldehyde **2** the imines **8**, while with two equiv. of **2** the (aminoethyl)oxadiazolines **10** are formed (Scheme 3). According to our own experiments in the reaction of one equiv. of benzaldehyde (**2a**) or its derivatives containing electron-attracting substituents (**2b–d**) imines **8a–d** formed which equilibrate in solution with the pyrimidines **9**. Both forms could be isolated in pure form and interconverted in solution. In contrast, in the case of cinnamaldehyde (**2g**) and benzaldehydes containing electron-releasing substituents (**2e, f**) only the open-chain imine tautomers (**8e–g**) could be detected[4f] both in solution and in the solid state.

In view of these findings[4b,f] reinvestigation of the structure **10** proposed for the product of **7** and two equiv. of the aldehydes[6] appears to be justified.

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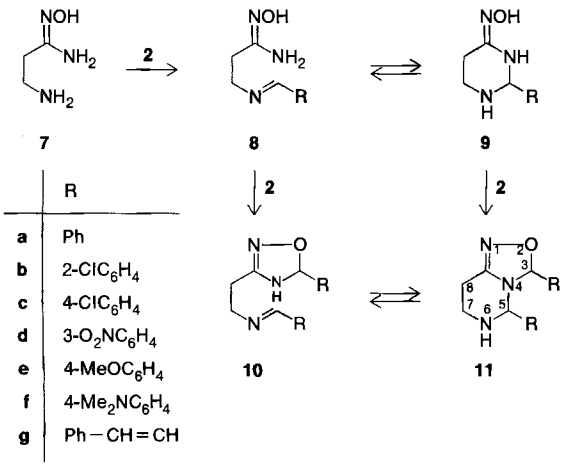
Scheme 3



In fact, when according to the literature[6] 3-aminopropionamide oxime (**7**) was heated with two equiv. of benzaldehyde either in a solvent or neat the obtained product proved to be not **10a**, but 5,6,7,8-tetrahydro-3,5-diphenyl-3*H*-[1,2,4]oxadiazolo[4,3-*c*]pyrimidine (**11a**), the first member of a new heterocyclic ring system. Its eventual formation was envisaged in the literature[6], but based on NMR and IR data this possibility was discarded. Note that the yield of **11a** is higher when a 10% excess of benzaldehyde is used. ^{1}H-, ^{13}C-, and ^{15}N-NMR as well as IR-spectral data all supported structure **11a**. Assignments were facilitated by comparison with spectra obtained earlier with compounds of a similar structure[4b–d,f]. In the ^{1}H-NMR spectrum of a freshly prepared solution in $CDCl_3$ of the white crystalline substance (m.p. 129–130°C; ref.[b] 129–130°C) signals for a $-CH=N-$ proton and a double triplet of the A_2X_2 type, characteristic of the $-CH_2CH_2-$ group, expected for structure **10a** were missing.

The methylene hydrogens are nonequivalent and instead of one single $-CH-$ doublet, as required by formula **10a**, two $-CH-$ singlets were visible. A $-CH=N-$ signal was also missing in the ^{13}C-NMR spectrum, giving way to two close $-CH-$ carbon signals. All these features favoured structure **11a** rather than **10a**. Clarification of the relative configuration of the chiral centers at C-3 and C-5 in **11a** was achieved by the observation of the time dependence of its NMR spectra. Decreasing intensity of the signals observed for the freshly prepared solution was accompanied first by the emergence of a second set of signals assignable to the Schiff base form **10a** and later by a third one characteristic of a stereoisomer of the starting material. Finally, a three-component equilibrium was established. The structure of the tautomers together with the relevant ^{1}H-, ^{13}C-, as well as tentative ^{15}N-NMR assignments are shown in Scheme 4, while the time course of the equilibration is documented in Table 1.

Scheme 4. Structure and ^{1}H-, ^{13}C-, and ^{15}N NMR data of the tautomers *cis*-**11a**, **10a**, and *trans*-**11a** (equilibrated $CDCl_3$ solution at 20°C; [a] assignments may be interchanged; [b] J = 6 Hz)

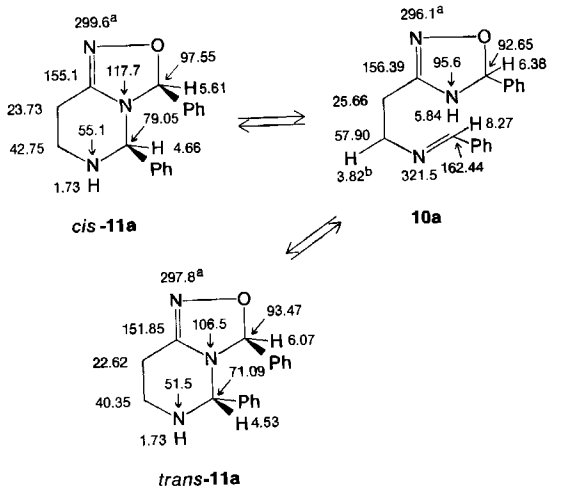


Table 1. Change of the ratios of the tautomers *cis*-**11a**, **10a**, and *trans*-**11a** with time after dissolution of *cis*-**11a** in $CDCl_3$ at 20°C

Time	*cis*-11a	10a	*trans*-11a
	%	%	%
5 min	100	--	--
2 h	68	27	5
7 h	59	27	14
22 h	52	27	21
144 h	51	24	25

The *cis* configuration of the originally isolated sample of **11a** involving the diaxial disposition of 3-H and 5-H as well as that for its *trans* stereroisomer having an equatorial 5-H and a quasi-axial phenyl group were based on ^{1}H and ^{13}C-NMR data with corroborative evidence from the ^{15}N-NMR spectra. Since ^{1}H-NMR signals could be unambiguously assigned for both stereoisomers DNOE experiments became feasible. Thus, irradiation of 5-H (δ = 4.69) in *cis*-**11a** resulted in a 14% enhancement of the signal of 3-H (δ = 5.61), while no such effect could be produced in the *trans* isomer. *γ-gauche* effects at C-3 and C-7 of the *trans* isomer can be explained by the quasi-axial orientation of the C-5 phenyl substituent.

Finally, the proposed structure for *cis*-**11a** was confirmed by X-ray crystallography (Figure 1).

The structures were also in agreement with the IR spectra. The solid-state spectrum (in KBr) of *cis*-**11a** showed only a single strong band in the range of 1700–1600 cm^{-1} at 1610 cm^{-1}. In a freshly prepared chloroform solution this band appeared at 1612 cm^{-1}, but after 2 h a second band emerged at 1645 cm^{-1}, originating from the C=N bond of the open-chain form **10a**. In the literature[6] two bands have been recorded in this region of the solution IR spectra from which an incorrect conclusion was drawn concerning the solid-state structure. This misassignment can be explained by equilibration prior to recording the spectra. It should be noted that misinterpretation of the NMR data cannot be

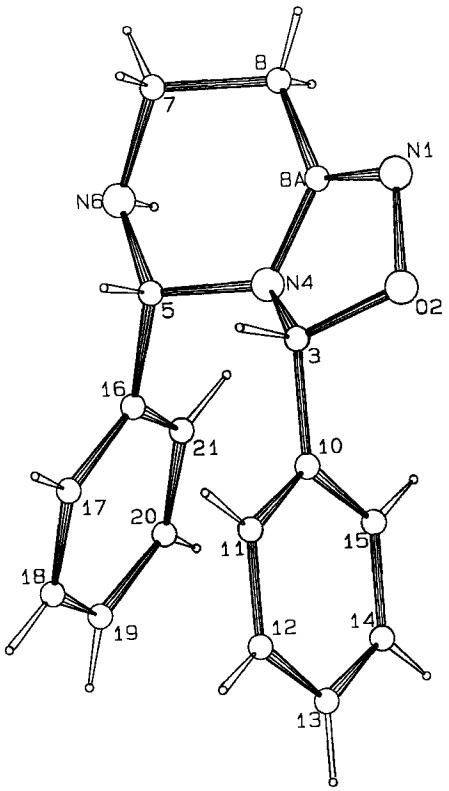


Figure 1. X-ray diagram of *cis*-**11a** with crystallographic atomic numbering. Some characteristic bond lengths and angles: N1–O2 1.460(2), N1–C8a 1.276(2), O2–C3 1.428(3), C3–N4 1.466(2), N4–C5 1.486(2), N4–C8a 1.387(3), C5–N6 1.453(2) N6–C7 1.465(3), C7–C8 1.528(3), C8–C8a 1.479(2) Å; O2–N1–C8a 104.8(3), N1–O2–C3 105.8(2), O2–C3–N4 (101.3(2), C3–N4–C5 118.1(2), C3–N4–C8a 102.5(2), C5–N4–C8a 120.2(2), C5–N6–C7 112.6(3), N1–C8a–N4 114.9(3), N1–C8a–C8 124.5(3)°

explained in this way since in solution the cyclic forms (*cis*- and *trans*-**11a**) always predominate over the open-chain form (**10a**) (Table 1). The triple tautomeric equilibrium is rather mobile as shown by a reversible shift in favour of the open-chain species in the equilibrated $CDCl_3$ solution on elevation of the temperature. On evaporation or precipitation it was always the readily crystallizing *cis*-**11a** which could be recovered. In this respect there is a marked difference as compared to the tautomeric system **8a–d** ⇄ **9a–d**, since with the latter treatment with different solvents permitted the isolation of both forms[4f].

Table 2. Tautomeric equilibrium ratios of the compounds *cis*-**11**, **10**, and *trans*-**11** at 20°C

No	R	*cis*-**11** %	**10** %	*trans*-**11** %	Solvent
a	Ph	51	24	25	$CDCl_3$
b	2-ClC_6H_4	57	28	15	$CDCl_3$
c	4-ClC_6H_4	55	22	23	$CDCl_3$
e	4-$MeOC_6H_4$	24	70	6	[D_6]DMSO
g	Ph-CH=CH	7	92	1	[D_6]DMSO

Similar to the reaction of **7** with two equiv. of benzaldehyde a triple tautomeric system could be observed in solution for the products resulting from the reaction of **7** with the aldehydes **2b, c, e, g**. The equilibrium ratio of the tautomers is shown in Table 2.

It can be seen that with 2- and 4-chlorobenzaldehyde, in agreement with the tendency reported in the literature[2b], the situation is similar to that with benzaldehyde. With anisaldehyde (**2e**) containing an electron-releasing methoxy group and especially with cinnamaldehyde (**2g**) it is the open-chain species (**10e, g**) which predominates. This may be partly due to the fact that owing to the insolubility of the compounds in the latter cases the solvent used was [D_6]DMSO. The relative configuration of the stereoisomers isolated in the crystalline form was for all three benzaldehyde derivatives (**11b, c, e**) *cis*, and the melting points of the products agreed with those reported[6]. With cinnamaldehyde the crystalline product was shown to be the open-chain species (**10g**), and this was the only case in this series when the original structural assignment[6] proved to be correct (Figure 2).

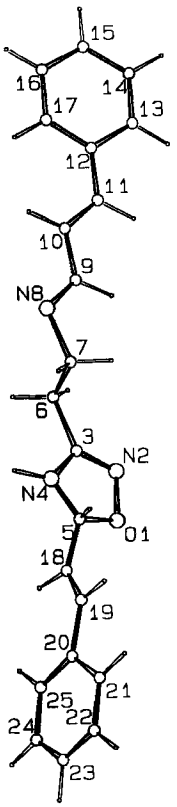


Figure 2. X-ray diagram of **10g** with crystallographic atomic numbering. Some characteristic bond lengths and angles: O1–N2 1.43(2), N2–C3 1.25(2), C3–C4 1.37(2), N4–C5 1.35(2), C5–O1 1.42(2), C6–C7 1.35(3), N8–C9 1.28(2), C10–C11 1.33(2), C18–C19 1.25(2) Å; N2–O1–C5 106(1), O1–N2–C3 104(1), N2–C3–C4 117(1), C3–N4–C5 105(2), O1–C5–N4 106(1)°

It ought to be emphasized that, in contrast to imine **8** or pyrimidine **9**[4f], in the reaction of **7** with two equiv. of aldehyde the formation of the pyrimidine ring of the bicyclic compounds **11a–c, e, g** was possible irrespective of the structure of the aldehyde. The oxadiazolopyrimidine **11** can obviously be formed not only directly from **9** (a process analoguous to the reaction **5**→**6**) (Scheme 2[4b]), but also via **10** (Scheme 3). The latter assumption is supported by the fact that the triple tautomeric systems were not only ob-

tained from the isolated pyrimidines **9a–c** and the imines **8a–c** but also from the imines **8e,g** by treating them with an additional equiv. of aldehyde despite the fact, that the latter exist, according to our studies, always in the open-chain form. An explanation for the formation of the condensed pyrimidines **11e,g** may be that the secondary amino group of oxadiazolines **10e,g** arising from **8e,g** and **2e,g** shows a greater tendency for the addition to the imino group than the primary amino group of the parent amide oximes.

Conclusions

The crystalline products isolated from the reaction of 3-aminopropionamide oxime (**7**) with two equiv. of an aromatic aldehyde are not, as claimed[6], the open-chain imines **10** but rather *cis*-3,5-disubstituted 5,6,7,8-tetrahydro-3*H*-[1,2,4]oxadiazolo[4,3-*c*]pyrimidines (**11a–c,e**), representatives of a new ring system. In the case of cinnamaldehyde the structure of the isolated product (**10g**) is as suggested in the literature. By solution-NMR studies we were probably the first to demonstrate a triple *endo*-type[3] ring-chain tautomerism involving addition of an amino group to a C=N bond, a transformation analogous to the mutarotation of sugars.

We are indebted to Dr. *L. Pusztay* for recording the IR spectra and to Dr. *I. Remport* for performing the microanalyses.

Experimental

IR: Zeiss Specord M-80. – ^{1}H, ^{13}C, and ^{15}N NMR: Jeol FX-100.

*cis-3,5-Disubstituted 5,6,7,8-Tetrahydro-3H-[1,2,4]oxadiazolo[4,3-c]pyrimidines cis-***11a–c,e** (General Methods)

a) To a suspension of **7**[7] (0.52 g, 5 mmol) in methanol (5 ml) the aldehyde **2a–c,e** (11 mmol) was added with shaking. With mild evolution of heat a solution was formed which was then kept in a closed flask at 80°C for 3 h. On cooling and scratching the product crystallized. After the addition of methanol (2 ml) and storing in a refrigerator for 4 d the product was filtered off, washed with some cold methanol and diethyl ether and recrystallized from ethanol.

b) **9a–c**[40] (5 mmol) and aldehyde **2a–c,e** (5.5 mmol) in methanol (5 ml) were treated as described under a).

c) **8a–c**[40] (5 mmol) and aldehyde **2a–c,e** (5.5 mmol) in methanol (5 ml) were treated as described under a).

Yields, melting points, IR and NMR spectra of the products (**11**) obtained by all three methods were identical and agreed also with those obtained for samples prepared by the method described in the literature[6] for structures **10a–c**. ^{1}H-, ^{13}C-, and ^{15}N-NMR data for **10a** and *cis*- and *trans*-**11a** are listed in Scheme 4, characteristic ^{1}H- and ^{13}C-NMR data for compounds **10b,c,e** and **11b,c,e** in Table 3. Yields, melting points, IR and analytical data for **11a–c,e** are compiled in Table 4.

Table 3. Characteristic ^{1}H- and ^{13}C-NMR data of compounds **10b,c,e**, *cis*-**11b,c,e,g**, and *trans*-**11b,c,e,g** (δ values, numbering of atoms according to Figures 1 and 2)

No	^{1}H NMR		^{13}C NMR		
10b	6.70 (5-H)	8.63 (10-H)	58.06 (C-8)	89.10 (C-5)	159.19 (C-10)
10c	6.36 (5-H)	8.22 (10-H)	58.01 (C-8)	92.00 (C-5)	161.41 (C-10)
10e	6.23 (5-H)	8.30 (10-H)	56.70 (C-8)	91.47 (C-5)	161.33 (C-10)
cis-**11b**	5.31 (5-H)	6.21 (3-H)	48.82 (C-7)	74.97 (C-5)	93.60 (C-3)
trans-**11b**	5.22 (5-H)	6.52 (3-H)	39.81 (C-7)	68.39 (C-5)	90.39 (C-3)
cis-**11c**	4.64 (5-H)	5.56 (3-H)	48.62 (C-7)	78.45 (C-5)	96.70 (C-3)
trans-**11c**	4.49 (5-H)	6.05 (3-H)	40.60 (C-7)	71.49 (C-5)	92.63 (C-3)
cis-**11e**	4.63 (5-H)	5.56 (3-H)	42.39 (C-7)	77.96 (C-5)	95.98 (C-3)
trans-**11e**	4.49 (5-H)	5.86 (3-H)	--	--	--
cis-**11g**	4.36 (5-H)	5.46 (3-H)	--	76.29 (C-5)	95.45 (C-3)
trans-**11g**	4.63 (5-H)	5.85 (3-H)	--	--	--

Table 4. Yields, melting points, IR-spectral and analytical data of *cis*-**11a,b,c,e**

No.	Yield % m.p. °C	ν_{max} (KBr) cm^{-1}	Formula (Mol. mass)	Calcd. Found C	H	N
cis-**11a**	64	3255, 2830,	$C_{17}H_{17}N_3O$	73.10	6.13	15.04
	130-133	2760, 2700, 1610	(279.3)	72.91	6.28	14.88
cis-**11b**	64	3305, 2950,	$C_{17}H_{15}Cl_2N_3O$	58.63	4.34	12.07
	134-135	2910, 2845, 1608	(348.2)	58.40	4.11	11.70
cis-**11c**	50	3292, 2960,	$C_{17}H_{15}Cl_2N_3O$	58.63	4.34	12.07
	129-133	2920, 2810, 1600	(348.2)	58.35	4.55	12.00
cis-**11e**	61	3260, 2900,	$C_{19}H_{21}N_3O$	67.24	6.24	12.38
	120-124	2815, 1603	(339.4)	66.94	6.14	12.18

*Crystal Data of cis-***11a**[8]: $C_{17}H_{17}N_3O$, M = 279.3. Monoclinic, a = 16.089(1), b = 5.682(1), c = 17.247(2) Å, β = 116.65(1)°, space group $P2_1/n$, Z = 4, V = 1409.1 Å^3, D_c = 1.317 g cm^{-3}. 3203 reflections, out of them 2891 unique, were collected with an Enraf Nonius CAD4 diffractometer, crystal size 0.25 × 0.25 × 0.40 mm, with Cu-K_α radiation (λ = 1.5418 Å), Θ_{range} = 1.5–75°, scan technique $\Theta/2\Theta$, μ(Cu-K_α, graphite monochromator) = 6.3 cm^{-1}. The structure was solved by SHELX-86[9] and refined by the SDP program package, R = 0.051, R_w = 0.050 for 2530 reflections [$I > 3\sigma(I)$], R = 0.06 for 2891 reflections. The weighting scheme was $w = 1/[\sigma^2(F_o) + 0.01\,F_o^2]$, the number of parameters refined 190, the highest residual electron density was 0.26 e/Å^3. The N–H hydrogen atom was taken from a difference Fourier map, all C–H hydrogens were calculated (C–H 0.95 Å) at the ideal geometrical positions, and the hydrogen atoms were included into the structure-factor calculations, but their positions were not refined. Atomic coordinates and equivalent B(eq) values with e.s.d's are given in Table 5.

3-[2-(Cinnamylideneamino)ethyl]-4,5-dihydro-5-styryl-1,2,4-oxadiazole (**10g**)

a) To a suspension of **7**[7] (0.52 g, 5 mmol) in methanol (5 ml) **2g** (1.49 g, 11 mmol) was added with stirring within 30 s. After standing at room temp. for 2 d and in the refrigerator for 4 d the crystals were filtered off, washed with some cold methanol and diethyl ether

to give the product (0.94 g, 57%), m.p. 136–139°C (from ethanol) (ref.[6] 133–136°C).

Table 5. Atomic coordinates and temperature factors [Å²] of *cis*-**11a** with e.s.d's. All atoms given were refined anisotropically

Atom	x/a	y/b	z/c	B(eq)
N(1)	.4369(1)	.3118(3)	.0805(1)	3.06(4)
O(2)	.38227(9)	.2140(3)	.12129(9)	3.19(4)
C(3)	.4296(1)	.0050(4)	.1646(1)	2.44(4)
N(4)	.5264(1)	.0665(3)	.18764(9)	1.99(3)
C(5)	.5962(1)	-.1262(3)	.2146(1)	2.02(4)
N(6)	.6756(1)	-.0704(3)	.1991(1)	2.37(4)
C(7)	.6483(1)	.0273(4)	.1124(1)	2.60(5)
C(8)	.5959(1)	.2591(4)	.1007(1)	2.78(5)
C(8a)	.5171(1)	.2182(3)	.1212(1)	2.34(4)
C(10)	.4076(1)	-.0535(4)	.2379(1)	2.26(4)
C(11)	.3606(1)	-.2602(4)	.2354(1)	2.85(5)
C(12)	.3388(1)	-.3153(4)	.3026(1)	3.34(6)
C(13)	.3646(1)	-.1650(5)	.3722(1)	3.53(7)
C(14)	.4122(1)	.0408(5)	.3753(1)	3.47(7)
C(15)	.4325(1)	.0970(4)	.3084(1)	2.81(5)
C(16)	.6277(1)	-.1844(3)	.3091(1)	2.04(4)
C(17)	.6020(1)	-.3947(4)	.3329(1)	2.46(4)
C(18)	.6298(1)	-.4482(4)	.4187(1)	2.92(5)
C(19)	.6854(1)	-.2933(4)	.4832(1)	3.15(5)
C(20)	.7124(1)	-.0829(4)	.4605(1)	3.13(5)
C(21)	.6829(1)	-.0282(4)	.3743(1)	2.46(4)

b) **8g**[4f] (1.09 g, 5 mmol) and **2g** (0.75 g, 5.5 mmol) were heated in methanol (5 ml) until dissolution. After cooling method a) was applied. Yield 1.24 g (75%), m.p. 137–140°C. Spectral data of the products obtained by methods a) and b) as well as in the literature[6] were identical. – IR (KBr): $\tilde{\nu}$ = 3150 cm^{-1}, 2860, 2820, 1630, 1610. – NMR: numbering of atoms according to Figure 2. – ^{1}H NMR ([D$_6$]DMSO): δ = 2.52 (t, *J* = 7 Hz, 2H, CH$_2$, 6-H), 3.70 (t, *J* = 7 Hz, 2H, CH$_2$, 7-H), 5.90 (dd, ABX, *J* = 1.5 Hz, CH–NH, *J* = –6.8 Hz, vic, 1H, 5-H), 6.22 (m, ABX, *J* = –6.8, vic, *J* = 15.7 Hz, *trans*, 1H, 18-H), 6.71 (m, ABX, *J* = 15.7/–0.4 Hz, CH–NH, 1H, 19-H), 6.93 (m, ABX, *J* = 16, *trans*, *J* = 7 Hz, vic, 1H, 10-H), 7.06 (m, ABX, *J* = 16, *trans*, *J* = 2 Hz, 1H, 11-H), 7.23 (d, *J* = 1.5 Hz, 1H, NH), 7.2–7.7 (m, 10H, Ar), 8.10 (m, ABX, d, separation *J* = 7 Hz, 1H, 9-H). – ^{13}C NMR ([D$_6$]DMSO): δ = 25.63 (C-6), 56.87 (C-7), 91.53 (C-5), 155.51 (C-3), 163.32 (C-9).

$C_{21}H_{21}N_3O$ (331.4) Calcd. C 76.13 H 6.39 N 12.68
Found C 76.26 H 6.26 N 12.40

Characteristic NMR data of small amounts of *cis- and trans*-**11g** formed in solutions of **10g** in [D$_6$]DMSO are shown in Table 3.

Crystal Data of **10g**[8]: $C_{21}H_{21}N_3O$, *M* = 331.4. Triclinic, *a* = 5.922(1), *b* = 8.319(1), *c* = 18.865(4) Å, α = 78.13(1), β = 87.13(2), γ = 81.02(1)°, space group $P\bar{1}$, *Z* = 2, *V* = 898.2 Å^3, D_c = 1.222 g cm^{-3}. 1852 reflections, out of them 1511 unique, were collected with an Enraf Nonius CAD 4 diffractometer, crystal size 0.07 × 0.10 × 0.23 mm, with CuK_α radiation (λ = 1.5418 Å), Θ_{range} = 1.5–50°, scan technique Θ/2Θ, μ(Cu-K_α graphite monochromator) = 5.7 cm^{-1}. We had difficulties in finding a suitable crystal, even the crystal selected for data collection was of poor quality, therefore there was no reason to collect data above Θ = 50°. The structure was solved by SEHLXS-86[9] and refined by SHELX-76, for 1266 reflections [$F > 3\sigma(F)$], *R* = 0.09, R_w = 0.11. The weighting scheme was $w = 4.9/[\sigma^2(F_o) + 0.001\ F_o^2]$, the number of parameters refined: 227, the highest residual electron density was 0.79 e/A^3. All hydrogens were calculated (d_{X-H} 0.95 Å) at the ideal geometrical positions, and they were riding with an overall isotropic temperature factor on the corresponding heavy atoms. Atomic coordinates and equivalent *B*(eq) values with e.s.d's are given in Table 6.

Table 6. Atomic coordinates and temperatures factors [Å²] of **10g** with e.s.d's. All atoms given were refined anisotropically

Atom	x/a	y/b	z/c	B(eq)
O(1)	.3759(9)	.9417(7)	.6458(3)	5.8(2)
N(2)	.267(1)	.9358(9)	.5803(4)	5.7(3)
C(3)	.387(2)	.817(1)	.5585(5)	7.9(5)
N(4)	.558(1)	.728(1)	.6031(4)	7.5(4)
C(5)	.529(2)	.790(1)	.6638(6)	8.4(5)
C(6)	.357(2)	.779(1)	.4783(5)	8.2(5)
C(7)	.219(2)	.662(1)	.4924(7)	9.6(5)
N(8)	.195(1)	.6096(9)	.4181(4)	6.3(3)
C(9)	.010(1)	.676(1)	.3845(5)	5.7(4)
C(10)	-.061(1)	.628(1)	.3228(4)	4.4(3)
C(11)	-.260(1)	.696(1)	.2920(4)	4.5(3)
C(12)	-.356(1)	.6672(9)	.2268(4)	4.1(3)
C(13)	-.573(1)	.746(1)	.2063(5)	5.1(3)
C(14)	-.671(1)	.727(1)	.1441(5)	5.8(4)
C(15)	-.547(2)	.630(1)	.0996(5)	5.9(4)
C(16)	-.332(2)	.547(1)	.1198(5)	5.8(4)
C(17)	-.235(1)	.5659(9)	.1825(4)	4.8(3)
C(18)	.699(2)	.806(1)	.7128(5)	5.2(4)
C(19)	.715(2)	.773(1)	.7802(7)	7.6(5)
C(20)	.877(2)	.814(1)	.8295(6)	5.4(4)
C(21)	.827(2)	.771(1)	.9024(7)	5.9(4)
C(22)	.958(2)	.807(1)	.9530(5)	6.9(5)
C(23)	1.141(2)	.884(1)	.9310(8)	7.0(6)
C(24)	1.193(2)	.926(1)	.8620(9)	7.2(4)
C(25)	1.060(2)	.893(1)	.8096(5)	5.8(4)

CAS Registry Numbers

2a: 100-52-7 / **2b**: 89-98-5 / **2c**: 104-88-1 / **2e**: 123-11-5 / **2g**: 14371-10-9 / **7**: 16750-43-9 / **8a**: 134940-53-7 / **8b**: 134940-54-8 / **8c**: 134940-55-9 / **8g**: 134940-64-0 / **9a**: 134940-56-0 / **9b**: 134940-57-1 / **9c**: 134940-58-2 / **10g**: 134940-63-9 / *cis*-**11a**: 134940-59-3 / *trans*-**11a**: 13440-66-2 / *cis*-**11b**: 134940-50-6 / *cis*-**11c**: 134940-61-7 / *cis*-**11e**: 134940-62-8 / *cis*-**11g**: 134940-65-1 / *trans*-**11g**: 135029-27-5

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