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SYNTHESIS OF 2,3-DIARYL-4-METHYLSULFONYLPYRROLO-[2,3-*b*]QUINOXALIN-2-ONES

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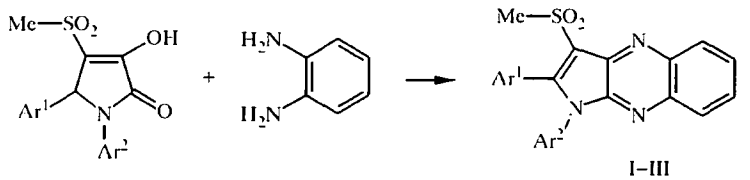
We have observed that when 1,5-diaryl-3-hydroxy-4-methylsulfonyl-3-pyrrolin-2-ones are fused with *ortho*-phenylenediamine at 190°C for 0.5 h, the reaction occurs at the carbonyl groups in the 2 and 3 position of the heterocycle, is accompanied by dehydrogenation, and leads to formation of 2,3-diaryl-4-methylsulfonylpyrrolo[2,3-*b*]quinoxalin-2-ones (I-III).



I-III

I, III $Ar^1 = C_6H_5$; II 4-MeC_6H_4; I, II $Ar^2 = C_6H_5$; III Ar^2 = 4-FC_6H_4

Compounds I-III are yellow-green crystalline materials which dissolve well in DMSO and DMF and, in contrast to the starting 1,5-diaryl-3-hydroxy-4-methylsulfonyl-3-pyrrolin-2-ones [1], do not give a cherry color with an alcoholic solution of iron(III) chloride.

In the PMR spectra of compounds I-III a group of lines from aromatic protons in the 7.15-8.30 ppm region and a singlet from the three protons of the methyl group at 3.50-3.53 ppm were observed.

In the IR spectra of compounds I-III, there are absorption bands from the sulfonyl group at 1137-1144 cm^{-1} and 1302-1318 cm^{-1} and an absorption band from the conjugated double bonds and aromatic protons in the 1539-1636 cm^{-1} region.

In the mass spectrum of compound I a molecular ion peak with *m/z* 417· $[M^+]$ and a fragmentary ion with *m/z* 338· $[M^+ - CH_3SO_2]^+$ were detected.

4-Methylsulfonyl-2,3-diphenylpyrrolo[2,3-*b*]quinoxalin-2-one (I). A mixture of 1,5-diphenyl-3-hydroxy-4-methylsulfonyl-3-pyrrolin-2-one (1.64 g, 5 mmol) and *ortho*-phenylenediamine (0.54 g, 5 mmol) were held at 190°C in a metal bath for 0.5 h. Then about 10 ml ethanol was added to the reaction mixture and the precipitate was filtered off. Yield 0.97 g (49%); mp 242-244°C (toluene). ^{1}H NMR spectrum (DMSO-d_6, HMDS): 3.53 (3H, s, CH_3SO_2); 7.20-7.80 (14H, m, 2Ph). IR spectrum (vaseline oil): 1144, 1318 (SO_2), 1540 (CN), 1636 (C=C). Found, %: C 69.25; H 4.27; N 10.58; S 8.14. $C_{23}H_{17}N_3O_2S$. Calculated, %: C 69.15; H 4.29; N 10.52; S 8.03.

3-(4-Methylphenyl)-4-methylsulfonyl-2-phenylpyrrolo[2,3-b]quinoxalin-2-one (II). Obtained similarly, yield 36%; mp 257-259°C (toluene.) ^{1}H NMR spectrum (DMSO-d_6, HMDS): 2.30 (3H, s, CH3); 3.50 (3H, s, CH_3SO_2); 7.15-8.30 (13H, m, Ar.) IR spectrum (vaseline oil): 1143, 1311 (SO_2), 1539 (CN), 1608 (C=C). Found, %: C 69.62; H 4.65; N 10.01; S 7.61. $C_{24}H_{19}N_3O_2S$. Calculated, %: C 69.71; H 4.63; N 10.16; S 7.76.

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2-(4-Fluorophenyl)-4-methylsulfonyl-3-phenylpyrrolo[2,3-*b*]quinoxalin-2-one (III). Obtained similarly, yield 26%; mp 259-260°C (toluene). ^{1}H NMR spectrum (DMSO-d_6, HMDS): 3.53 (3H, s, CH_3SO_2); 7.51 (13H, m, Ar). IR spectrum (vaseline oil): 1137, 1302 (SO_2), 1539 (CN); 1605 (C=C). Mass spectrum: *m/z* (*I*, %): 417 (27.63) $[M]^+$, 338 (59.46) $[M^+ - CH_3SO_2]^+$. Found, %: C 66.12; H 3.92; N 10.12; S 7.60. $C_{23}H_{16}FN_3O_2S$. Calculated, %: C 66.17; H 3.86; N 10.07; S 7.68.

The ^{1}H NMR spectra were recorded on a Bruker AM-300 in DMSO-d_6, internal standard HMDS. The IR spectra were measured on a UR-20 in vaseline oil. The mass spectra were obtained on a MAT-311A (40 eV) spectrometer.

REFERENCES

1. A. V. Kataeva, V. L. Gein, L. F. Gein, and Z. G. Aliev, *Zh. Obshch. Khim.*, **69**, No. 4, 697 (1999).