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SYNTHESIS OF A NEW HETEROCYCLIC SYSTEM, 1,2,3,7-TETRAAZAPYRENE

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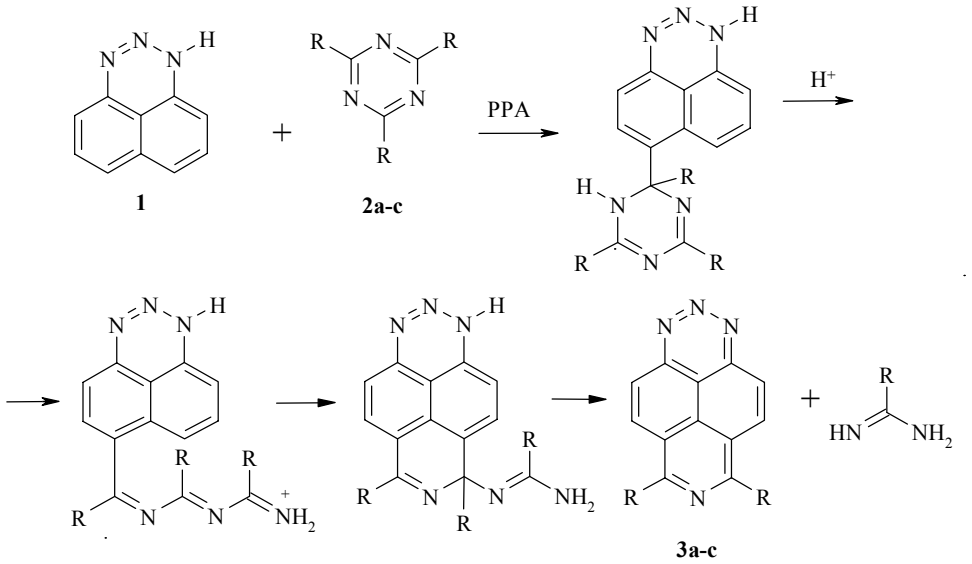
In previous work [1], we developed a method for the acylation (formylation) of perimidines based on their reaction with 1,3,5-triazines **2** in PPA. We unexpectedly found that the use of 1H-naphtho[1,8-*de*][1,2,3]triazine (1,2,3-triazaphenalene) (**1**) as the substrate in the reaction with substituted 1,3,5-triazines leads to a change in the direction of this reaction. Thus, we discovered that heating **1** (1 mmol) with 1,3,5-triazines (1.5 mmol) in 3-4 g PPA* for 1.5 h at 70°C and then for 3 h at 100°C (**2a**), 140°C (**2b**), or 150°C (**2c**) (isolation common for such reactions) leads to previously unreported 1,2,3,7-tetraazapyrenes **3** in 55-64% yield. The reaction probably proceeds through the following sequence of steps:



2,3 a R = H, **b** R = Me, **c** R = Ph

* The sample of PPA used was prepared according to Uhlig [2] and contained 86% P_2O_5

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The ^{1}H NMR spectra were taken on a Bruker WP-200 spectrometer at 200 MHz using TMS as the internal standard.

1,2,3,7-Tetraazapyrene (3a). Yield 0.132 g **(**64%); mp 212-214°C (ethyl acetate). ^{1}H NMR spectrum in DMSO-d_6, δ, ppm (*J*, Hz): 8.35 (2H, d, *J* = 9.5, H-5,9); 8.92 (2H, d, *J* = 9.5, H-4,10); 9.83 (2H, s, H-6,8). Found, %: C 70.06; H 2.86; N 27.08. $C_{12}H_6N_4$. Calculated, %: C 69.90; H 2.93; N 27.17.

6,8-Dimethyl-1,2,3,7-tetraazapyrene (3b). Yield 0.129 g (55%); mp 192-194°C (ethyl acetate). ^{1}H NMR spectrum in $CDCl_3$, δ, ppm (*J*, Hz): 3.49 (6H, s, CH_3); 8.40 (2H, d, *J* = 9.5, H-5,9); 8.81 (2H, d, *J* = 9.5, H-4,10). Found, %: C 71.92; H 4.22; N 23.86. $C_{14}H_{19}N_4$. Calculated, %: C 71.78; H 4.30; N 23.92.

6,8-Diphenyl-1,2,3,7-tetraazapyrene (3c). Yield 0.208 g (58%), mp 205-207°C (ethyl acetate). ^{1}H NMR spectrum in $CDCl_3$, δ, ppm (*J*, Hz): 7.61 (6H, m, 3,4,5-C_6H_5); 7.96 (4H, d, *J* = 7.4, 2,6-C_6H_5); 8.33 (2H, d, *J* = 9.5, H-5,9); 8.79 (2H, d, *J* = 9.5, H-4,10). Found, %: C 80.63; H 3.88; N 15.49. $C_{24}H_{14}N_4$. Calculated, %: C 80.43; H 3.94; N 15.63.

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