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Research Article

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Synthesis and structural elucidation of a new series of *s*-triazines derivatives

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ABSTRACT

6-amino Indazole condensed with trichloro s-triazine. Finally various aromatic amines derivatives were allowed to react and the product were characterized by conventional and instrumental methods. Their structures were determined.

Keywords: Synthesis**,** *s*-Triazine derivatives, Structural Elucidation.

INTRODUCTION

Nitrogen containing heterocycles play vital role in any industries. Among them 1,3,5-triazine represent a widely used lead structure with multitude of interesting application in numerous fields[1]. Several derivatives of *s*-triazine show antibacterial[2] ,antimicrobial[3] and herbicidal activities[4]. The replacement of a chlorine atom in cynuric chloride by basic group is greatly facilitated by the ring nitrogen atom of the symmetrically built *s*-triazine nucleus. 2,4,6 -trichloro -*s*-triazine derivatives prepared[5,6] by replacement of one chlorine atom at 0-5°C, second one at 35-45°C and third one at 80-100°C.

EXPERIMENTAL SECTION

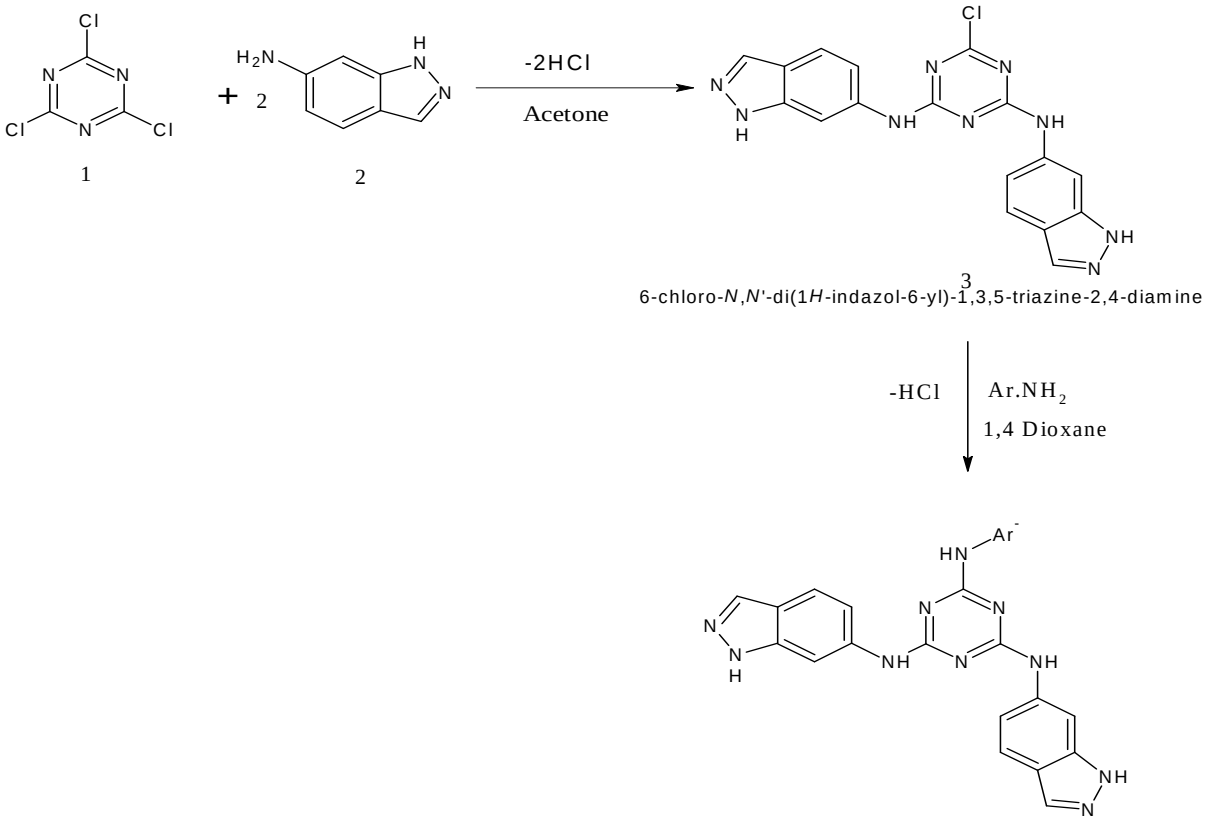
The reagent grade chemicals were obtained from commercial sources and purified by either distillation or recrystallization before use. Purity of synthesized compounds has been checked by thin layer chromatography. Melting points were determined by open capillary method and are uncorrected. IR spectra are recorded on FT-IR Bruker with KBr disc. ^{1}H NMR spectra are recorded in DMSO-d6 on a Bruker DRX-400 MHz using TMS as internal standard. The chemical shift are reported as parts per million(ppm) and mass spectra were determined on Jeol-SX-102(FAB) spectrometer.

Preparation of 6-chloro-*N*,*N*'-di(1*H*-indazol-6-yl)-1,3,5-triazine-2,4-diamine

In a conical flask, cyanuric chloride (0.01 mol) was taken acetone (25 mL) and 1*H*-indazol-6-amine (0.02 mol) was added to it. To this mixture 10% NaHCO3 was added drop wise at room temperature. The solution was stirred for 4 hours. The reaction mixture was poured onto crushed ice with constant stirring. The solid was sfiltered and washed with water. The product was recrystallized from acetone.

Preparation of N^2-(4-nitrophenyl)-N^4-N^6 bis(1*h*-indazol-6-yl)-1,3,5-triazine-2,4,-diamine

In a conical flask 6-chloro-*N*,*N*'-di(1*H*-indazol-6-yl)-1,3,5-triazine-2,4-diamine (0.01 mol) and 1,4 -dioxane (20 mL) was taken. To this mixture, p-nitro Amine (0.01 mol) was added. The PH was adjusted neutral by adding 10% NaHCO3. Then the reaction mixture was refluxed for 6 hrs. The reaction mixture was poured onto crushed ice with constant stirring. The solid was filtered and washed with water. The product was recrystallized from methanol. Their physical constant data are given in Table-1 and synthetic scheme in Figure-1.



Scheme-1

Figure-1. Synthesis route to *s*-triazine derivatives

Table-1. Physical constants and elemental analysis of *s*-triazines

Comp. No.	Ar-	Molecular Formula	M.P °C	Yield %	% of C Found, (calcd.)	% of H Found, (calcd.)	% of N Found, (calcd.)
SP_X-1	4-NO_2-C_6H_4	$C_{23}H_{17}N_{11}O_2$	235	76	57.64 (57.62)	3.58 (3.57)	32.16 (32.14)
SP_X-2	4-CH_3-C_6H_4	$C_{24}H_{20}N_{10}$	230	72	64.28 (64.27)	4,47 (4.49)	31.24 (31.23)
SP_X-3	3,4-$(Cl)_2$-C_6H_3	$C_{23}H_{16}Cl_2N_{10}$	260	74	54.89 (54.88)	3.22 (3.20)	27.85 (27.83)
SP_X-4	3-NO_2-C_6H_4	$C_{23}H_{17}N_{11}O_2$	265	76	57.63 (57.62)	3.58 (3.57)	32.16 (32.14)
SP_X-5	2-OH-4-$NO_2C_6H_3$	$C_{23}H_{17}N_{11}O_3$	270	70	55.77 (55.76)	3.48 (3.46)	31.12 (31.10)
SP_X-6	2-OH-C_6H_4	$C_{23}H_{18}N_{10}O$	280	74	61.35 (61.33)	4.05 (4.03)	31.07 (31.09)
SP_X-7	2-$C_4H_3N_2$	$C_{21}H_{16}N_{12}$	279	70	57.80 (57.79)	3.72 (3.70)	38.50 (38.51)
SP_X-8	2-Cl-C_6H_4	$C_{23}H_{17}ClN_{10}$	283	75	58.92 (58.91)	3.66 (3.65)	29.88 (29.87)
SP_X-9	3-Cl-C_6H_4	$C_{23}H_{17}ClN_{10}$	225	70	58.93 (58.91)	3.66 (3.65)	29.88 (29.87)
SP_X-10	2,4,5-$(Cl)_3$-C_6H_2	$C_{23}H_{15}Cl_3N_{10}$	230	77	51.38 (51.37)	283 (2.81)	26.05 (26.04)
SP_X-11	2-OCH_3-C_6H_4	$C_{24}H_{20}N_{10}O$	239	75	62.07 (62.06)	4.35 (4.34)	30.17 (30.16)
SP_X-12	2,4-$(NO_2)_2C_6H_3$	$C_{23}H_{16}N_{12}O_4$	245	79	52.68 (52.67)	3.09 (3.08)	32.03 (32.05)
SP_X-13	2,4-$(Cl)_2$-2 NO_2-C_6H_2	$C_{23}H_{15}Cl_2N_{11}O_2$	253	77	50.37 (50.38)	2.77 (2.76)	28.12 (28.10)
SP_X-14	3-Cl-6-OH-C_6H_3	$C_{23}H_{17}ClN_{10}O$	259	79	56.99 (56.97)	3.51 (3.53)	28.90 (28.89)
SP_X-15	3-Cl-4-F-C_6H_3	$C_{23}H_{16}ClFN_{10}$	265	77	56.75 (56.74)	3.33 (3.31)	28.79 (28.77)

Spectra study of N^2-(4-nitrophenyl)-N^4-N^6 bis(1*h*-indazol-6-yl)-1,3,5-triazine-2,4,-diamine
FT-IR (KBr) cm^{-1} : 3024(-N-H Str., Sec. amine), 1573(C=N Str., Sec. amine), 1473(C=N Str., ter. amine), 698 (m-sub. Bend. Vib.), 860(p-sub. Bend. Vib.) ^{1}H NMR: 7.92, 7.93δ (S, C-NH-, 2H), 6.62-7.92 (m, Ar-H, 12H), 2.53-2.55(s, 3H, -N**H**-),
MS: m/z. 480 [M+1].

RESULTS AND DISCUSSION

Various s-Triazine derivatives SP_X 1-15 were prepared using s-Triazine with 6-amino Indazole and Finally various aromatic amine replace third chlrine and form N^2-(4-nitrophenyl)-N^4-N^6 bis(1*h*-indazol-6-yl)-1,3,5-triazine-2,4,-diamine. All the compounds synthesized were adequately characterized by their elemental analyses and spectral IR, ^{1}H-NMR and Mass Spectra.

CONCLUSION

As outline in Scheme-1, an important novel s-Triazine derivatives, N^2-(4-nitrophenyl)-N^4-N^6 bis(1*h*-indazol-6-yl)-1,3,5-triazine-2,4,-diamine has been synthesized. All the structure of the above compounds were in good agreement with Spectral and Analytical data.

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REFERENCES

[1]. A. Rosowsky, S.F. Queener, *J. Med. Chem.*, **2004**, 47, 1475.
[2]. A.S. Gajare, M.S. Shingare, *Indian J. Chem.*, **1998**, 37B, 510.
[3]. P.S. Desai, K.R. Desai, *J. Indian Chem. Soc.*, **1994**,77, 155.
[4]. N. Nishimura, A. Kato, *Carbohyd. Res.*, **2001**, 77, 331.
[5]. D.W. Kaiser, J.T.Thurston, J.R. Dudley, F.C. Schaefer, D. Holm-Hansen, *J. Am. Chem. Soc.*, **1951**,73, 2984.
[6]. R.B. Patel, K.H. Chikhalia, *J. Indian Chem. Soc.*, **2003**, 80, 138.