PhytoChem & BioSub Journal Vol. 9(1) 2015
ISSN 2170-1768
CAS-CODEN:PBJHB3

PCBS Journal
ISSN 2170-1768

PhytoChem & BioSub Journal

2015
Vol. 9 No. 1

Synthesis 1, 3-*bis* (4-bromophenyl)-5-isopropyl-1, 3, 5-triazacyclohexane

Leila Lefrada*, Ahsen Bouchemma, Mustapha Bouhenguel, Mahmoud Chabbah & Amel Farahti

Laboratory of Applied Chemistry and Materials Technology, Faculty of Exact Sciences, Department Material Science, University Larbi Ben M'hidi of Oum El Bouaghi, Rue de Constantine, 04000, Algeria.

Received: July 14, 2014; Accepted: January 23, 2015
Corresponding author Email aliel_2011@yahoo.fr

DOI:10.163.pcbsj/2015.9.1.18

Abstract *Condensation of an isopropylamine and an 4-bromoaniline with formaline in basic solution to give 1, 3-bis (4-bromophenyl)-5- (isopropyl)- 1, 3, 5- triazicyaclohexane. Through the interaction of rapid Schiff base, Structures of this compound have been elucidated by spectroscopic methods; IR, ^{1}H NMR, ^{13}C NMR. Their purities were confirmed by elemental analyses.*

***Key Words*:** Condensation , isopropylamine, 4-bromoaniline

1. Introduction

The formation of 1, 3, 5-triazacyclohexane from primary amines and formaldehyde has been known for more than one hundred years [1]. The different triazines were synthesized in the laboratory according to the procedure described elsewhere [2]. The 1, 3, 5-triazacyclohexane are the subject of several structural studies considering, the use in the industrial chemistry which can be used as ligands for the preparation of new complexes that can be served as catalyst in the polymerization and trimerization of olefines [3]. However, interest in 1, 3, 5-triazacyclohexane as ligand seems to be growing rapidly [4] .

2. Experimental

2.1. Instrumentation

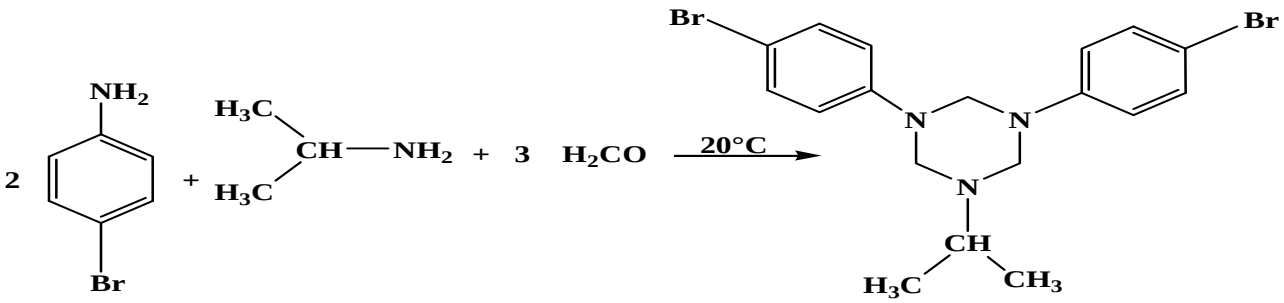
Purity of the compounds were checked by thin layer chromatography (TLC) using CH_2Cl_2:*n*-hexane (1:1). IR spectra were prepared on the Mattson Galaxy series FT-IR 5000 spectrophotometer using KBr discs. NMR spectra were recorded on Bruker spectrophotometer (250 MHz) in CDCl3 using TMS as an internal standard.

2.2. Synthesis

A stirred solution of (10 mmol, 1.72g) 4-bromoniline and (20 mmol, 1.182g, 1.64 ml) isopropylamine with potassium hydroxide (35 mmol, 1.964 g) in water 15 ml was added formaline (37%, 7.2mL, 36 mmol) was added dropwise. [5]. the reaction mixture was stirred hang 2 days at room temperature. The solution is condensed to 6 mL and left another night. After evaporating the solvent, recrystallization from hexane Yield: 91% (3.99g), M.p.: 114-115°C. IR (KBr, ν, cm-1): 2925.8(C-H), 1583.4 -1498.4 (C=C), 1276.8(C-N), 1136.0 (C-Br), 758.0 (C-H, Ar). 1H NMR (500 MHz, CDCl3): 1.15 (d, 6H, $C\underline{H}_3$), 3.04 (s, C_2H_6, $C\underline{H}$) , 4.4 (s, 4H, C_2H_5-N-$C\underline{H}_2$-N-Ar), 4.7 (s, 2H, Ar-N-$C\underline{H}_2$-N-Ar) 6.8-7. (m, 8H, Ar) [6]. ^{13}C-NMR (100 MHz, $CDCl_3$) 19.96- 20.35 ($\underline{C}H_3$-CH), 49.26 (C_2H_6-$\underline{C}$H-N), 53.977 (C_2H_5-$\underline{C}H_2$-N), 68.26 (C_3H_7-N-$\underline{C}H_2$-N-Ar), 71.12 (Ar-N-$\underline{C}H_2$-N-Ar), 112.97 ($\underline{C}$-Br) 119.10-132.14 ($\underline{C}$H=C-), 148.38 (N-$\underline{C}$=).

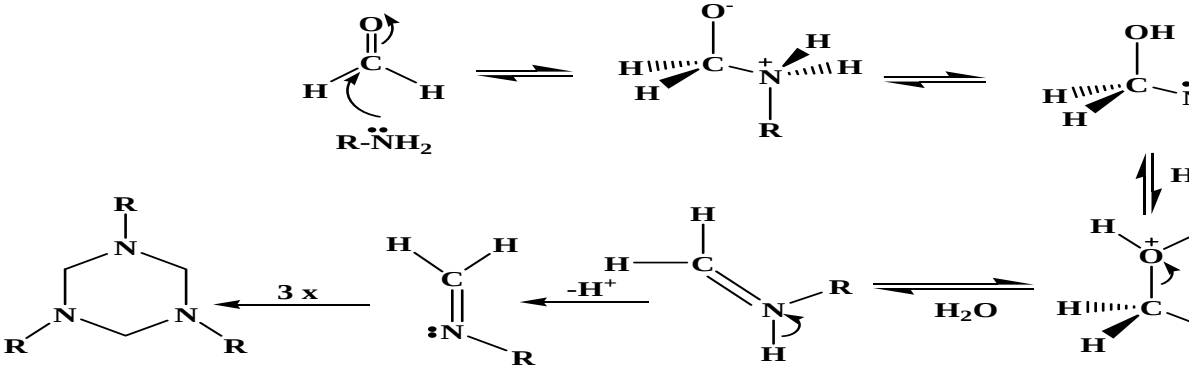
3. Results and discussion

The Unsymmetrically Substituted triazinane Such as 1, 3-bis (4-bromophenyl)-5- (isopropyl)-1, 3, 5- triazacyclohexane, It was prepared from the condensation reaction of isopropylamine and 4-bromoaniline with formaldehyde [6]. (Scheme 1), This compound is stable at room temperature and high yield (95%) with a transparent color



Scheme 1

The mechanism of interaction is the production of Schiff base, which polymerize to give 1, 3, bis(4-bromophényle)-5- (isopropyl)- 1, 3, 5- triazacyclohexanes (Scheme 2)



Scheme 2

Structure of compound have been elucidated by IR, ^{1}H NMR and ^{13}C NMR (2D, J-mod, HSQC) measurements. Their spectrashowed a strong band for the (C-Br) group at (1662-1658cm^{-1}), a band at (1583.4 -1498.4 cm^{-1}) for C=C and (758.0 cm^{-1}) for C-H, Ar. In the ^{1}H NMR. the six hydrogen atoms appear when you 1.15 ppm and relate with One atom of hydrogen to give Binary form, One atom of hydrogen 3.04 ppm attached to the 6-H To give the form of seven**,** Triazacyclohexanes ring hydrogen atoms appear when 4.4-4.7 ppm unilaterally And hydrogen atoms of the aryl ring appear when 6.8-7 ppm multi. And in the ^{13}C NMR, The carbon atoms of the isopropyl group appear at 19.96, 2035, 49.26, ppm, The carbon atoms of the group appears at the 1, 3, 5 triazacyaclohexane 68.26 – 71.12 ppm And carbon atoms of the aryl group appears at 119.10 , 132.14 , 148.38 ppm, The carbon ring aryl which has a bromine atom appears when it is 112.96 ppm. The carbon ring aryl which has a bromine atom appears when it is

4. Conclusion

We have Synthesis and characterization of new unsymmetrical 1, 3, 5- triazacyclohexane. The synthesis was starting from condensation of isopropylamine and an 4-bromoaniline with formalineand The new 1, 3-bis (4-bromophenyl)-5- (isopropyl)- 1, 3, 5- triazacyclohexane described in this paper are very stable compounds, a property which may render them especially useful substances ligands for the preparation of new complexes that can be served as catalyst in the polymerization and trimerization.

Acknowledgement
We thank the Mustapha. Bouhenguel director of the laboratory of applied chemistry and materials technology of the University Larbi Ben M'hidi of *Oum El Bouaghi,* Algeria.

References

[1]. Francimont, A. ; Van Erp, H. ; *Rec.trav. chim*, 1896, *15*.

[2]. Miller J.G., Wagner E.C., *JACS*, 54 (1932) 3698

[3]. Murray V. Baker, Mariac. Dalermo, Brianw. Skelton, Allan H. White, Aust. J.chem, 52, 1999

[4]. Guide, S.; Phd Thesis, Synthesis and Coordination Chemistry of Traizacyclohexane and Orthoamides, P11. 1999. Berline

[5]. Bouchemma, A. ; Peter, H. M. ;George, A. S. ;J Chem. Soc. Prans. 1989, Issue 1, 585-586.

[6]. Latreche, S. ; Bouchemma, A. ;Bouacida, S. ; Bouhenguel, M. ; Mousser, A. ; *Acta Cryst.* (2006). E62, o4676-o4678.