International Journal of ChemTech Research
CODEN(USA): IJCRGG ISSN : 0974-4290
Vol.2, No.3, pp 1856-1859, July-Sept 2010

Applications of Green Chemistry in Organic Synthesis

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Abstract: Green chemistry is the new and rapid emerging field of chemistry. Its growing importance is in utilization of maximum possible resources in such a way that, there is negligible or minimum production of chemical waste. It is one of the best alternatives for traditional chemical synthesis process. Few derivatives of acetanilide (compounds I- IV) were synthesized by conventional method as well as by green chemistry method. By applying the green synthesis method, we have not only avoided the use of acetic anhydride which is hazardous one but also the formations of by products are avoided. The atom economy was calculated on the basis of molecular weight of desired product and it was found to be in the range of 72% to 82% which signifies the utility of green synthesis method.
Key words: Green synthesis, green chemistry, acetanilide, atom economy.

Introduction :[1,2]

'Green Chemistry' is the new branch of chemistry which involves pulling together tools, techniques and technologies. It is helpful to chemists and chemical engineers in research, development and production for development of more eco-friendly and efficient products which may also have significant financial benefits. It is now going to become an essential tool in the field of synthetic chemistry. The development of Green Chemistry redefines the role of a solvent: "*An ideal solvent facilitates the mass transfer but does not dissolve*". In addition, a desirable green solvent should be natural, nontoxic, cheap and readily available with additional benefits of aiding the reaction, separation or catalyst recycling. Of the various principles of green chemistry, the important one is maximizing the Atom Economy which evaluates the efficiency of chemical transformation and is calculated as:

% atom utilization [3]

$$= \frac{\text{Molecular weight of desired product}}{\text{Molecular weight of (desired product + waste product)}} \times 100$$

In the present study, few derivatives of acetanilide (I-IV) are synthesized by conventional method as well as green synthesis method. The synthesized compounds are characterized by their physical constants and FTIR. Both the method gives the desired products, but by applying the green synthesis method, we can able to avoid the use of acetic anhydride and formation of by products. Moreover, the atom economy was obtained in the range of 72% to 82% which indicates the complete use of chemicals. Thus, concept of green chemistry can be applied to various synthetic methods. This may leads to generation of eco friendly synthetic chemistry.

Materials and Method:

Apparatus:

The melting points were determined by open capillary method and are uncorrected.

Infrared spectra were recorded on FTIR 8400s Shimadzu using KBr.

Chemicals and Reagents:

Aniline, p-chloroaniline, p-toluidine, p-nitroaniline, acetic anhydride, conc. HCl, sodium acetate, glacial acetic acid, zinc dust and methylated spirit are from Loba Chem Pvt. Limited, Mumbai. All solvents were distilled before use and dried whenever required.

Synthesis of compounds (I-IV) by conventional method: [4, 5]

In a 250 ml beaker containing 125 ml of water, 4.6 ml of conc. HCl and 5.1 g of aniline / substituted anilines were introduced. Stirred until all the anilines passes completely into solution. To the resulting solution, 6.9 g (6.4ml) of redistilled acetic anhydride was added and stirred until it was dissolved. Poured immediately in a solution of 3.8 g of crystalline sodium acetate in 25 ml of water. Stirred vigorously and cooled in ice. Filtered the acetanilide and substituted acetanilides with suction, washed with 10 ml water, drained well and dried upon filter paper. The crude products were recrystallized from boiling water and methylated spirit.

Non green component: Acetic anhydride leaves one molecule of acetic acid unused.

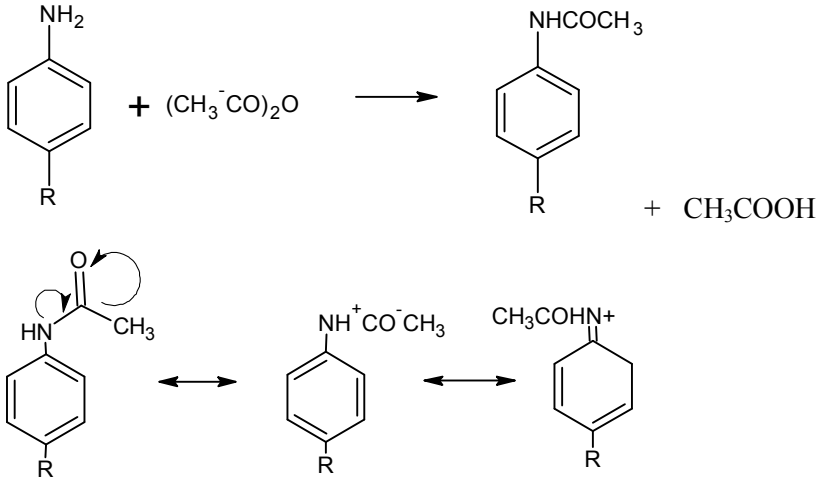
Synthesis of compounds (I-IV) by green chemistry method: [6]

A mixture of aniline / substituted anilines (3.3g) and zinc dust (0.16g) in acetic acid (10ml) in 100 ml round bottom flask was heated over a gentle flame using water condenser. Heating was continued for about 45 min., the reaction mixture was then carefully poured in cold water (33ml) in 250ml beaker with vigorous stirring. The shining crystals of product were separated slowly. After 15 min, crystals were collected by filtration. The solid crystals were washed over the Buchner funnel with water and product was dried and crystallized in boiling water.

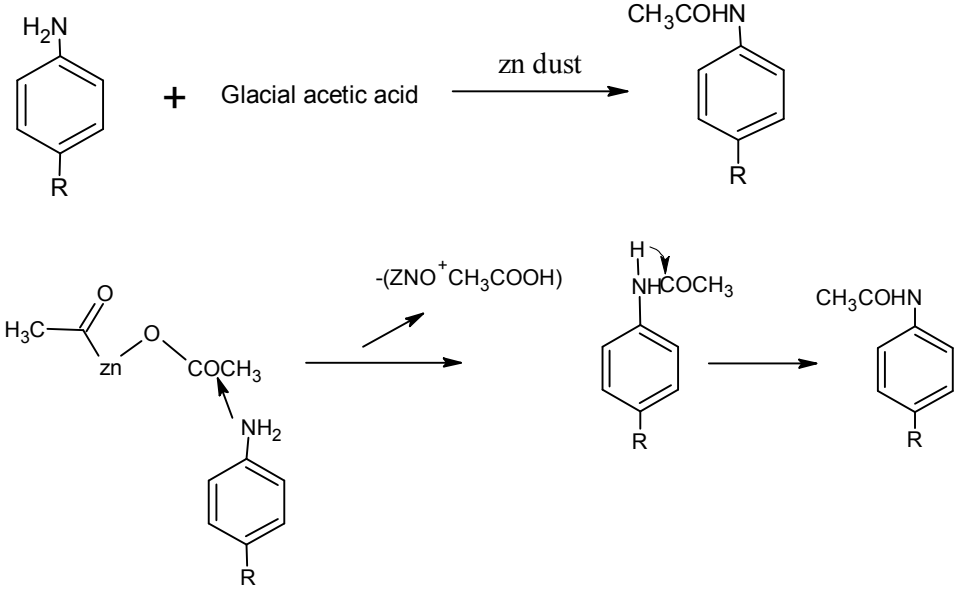
Green context: Minimize waste by-products, avoids use of acetic anhydride.

Scheme of Synthesis

Scheme of Synthesis and Mechanism by conventional method : [4, 5]



Scheme of Synthesis and Mechanism by green chemistry method : [6]



Results and Discussion

The synthesis of acetanilide & its derivatives was carried out successfully by using both conventional method as well as green chemistry method. The synthesized products were recrystallized and melting point was taken which are compatible with the reported melting points. The percent yield obtained by green chemistry method was found to be more than that of conventional method. All the compounds were characterized by FTIR which shows the presence of aromatic ring (3055-3122 cm^{-1}), amine group (3275-3481 cm^{-1}), amide (1631-1676 cm^{-1}) that characterized the said compounds. The atom economy was calculated on basis of the molecular weight of desired product and the molecular weight of all the products. From this calculation, it was seen that the atom economy is more in case of green chemistry than by the conventional method of synthesis. The found values signify the utility of method in which atom economy was obtained in the range of 70% to75%. The detail results are tabulated.

Table

Comp. No.	R	Green Synthesis Method			Conventional Method		Atom Economy
		%Yield	M. P. (^{O}C)	FTIR (cm^{-1})[7]	%Yield	M. P. (^{O}C)	
I	-H	79.78%	112°C	Aromatic- 3072 NH-3275 Amide-1676 Methyl-1448	55.66%	114°C	69.92 %
II	$-CH_3$	82.22%	146°C	Aromatic- 3122 NH-3290 Amide-1662 Methyl-1454 Methyl-1402	76 .67%	148-149° C	71.29 %
III	$-NO_2$	72.09%	210-212° C	Aromatic-3055 NH-3481 Amide-1631 Methyl-1444 Nitro-1402	64.78%	215-216°C	75.00 %
IV	-Cl	76.00%	182-183°C	Aromatic-3066 NH-3304 Amide-1664 Methyl-1371 Chloro-707	59.67%	179°C	73.34 %

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