Synthesis of Heterocyclic Compounds from Alpha- Beta Unsaturated Carbonyl Compounds

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Abstract: This study include the preparation of 1,3-diacetylindole from the reaction of indole (with acetic anhydride in presence of acetic acid as acidic media). The compound N-acetyl indole was prepared from the reaction of indole and acetic anhydride and the compound N-acetophenonindole was prepared from the reaction of α-chloroacetophenone and indole. These three compounds having an alpha acedic hydrogen which could be used in the synthesis of chalcones (H2-H8) using the following carbonyl compounds (4-nitrobenzaldehyde, 2-chlorobenzaldehyde, 4-N, N-dimethylaminobenzaldehyde, 2,5-hexanedione, 3-acetyl indole and acetone) through Aldol condensation to obtain α,β-unsaturated carbonyl compounds. On treatment of 1,3-diacetyl indole with (10%) potassium hydroxide solution, the amid group will be hydrolysis to the amine group in position (I), so the acetyl group in the indole will be the center of the reaction. The prepared chalcones, has been used in the synthesis of many heterocyclic compounds, when react with biurate give substituted pyrimidinone containing the hexamembered ring (H9-H15). The reaction of chalcone with N-bromosuccinamide gives the monobromo derivatives (H18-H24). The reaction with phenyl hydrazine give the pyrazoline of the pentamembered ring (H25-H31). On the reaction with hydrogen peroxide giving the oxirane (H32-H38).which suffering from the expansion ring through the treatement with hydrazine hydrate gives pyrazoline diole compounds (H39-H45). The reaction with methyurea gives substituted pyrimidinone compounds of hexamembered ring (H46-H52). The synthesis triazole compounds (H53) which prepared from the reaction of 1,3,4-oxadiazole- 5-thiole with hydrazine hydrate reacting (N-acetylinholde, 1,3-diaacetylindolde) to obtain the imines (H55,H56) respectively. The chalcone (H58) was prepared from the reaction of N-acetophenone indole with 2-chlorobenzaldehyde, this synthesized chalcone was reacted with triazole to obtain the schiff’s base (H59). All the synthesized compounds were identified using the available physical and spectroscopic methods [m. p., color change, (IR, UV and 1H- NMR spectra) and some theoretical calculations].

Introduction
α, β-Unsaturated ketones are convenient and easily available starting materials or intermediates for the synthe-sis of a wide variety of heterocyclic compounds. The α,β-enone unit is favourable for dipolar cycloaddition reac-tions with various reagents affording heterocyclic com-pounds of different ring sizes with one or more heteroatoms. Their reactions with dinucleophiles provide impres-sive and useful heterocyclic ring systems as well. Among the α,β-unsaturated ketones, chalcones and their analogues have a prominent place as starting materials for the synthe-sis of, first of all, nitrogen-containing heterocyclic com-pounds. Such reactions have been reviewed in several accounts [1-5].
Utilization of the related exocyclic α, β-unsaturated ketones for such purposes made possible the synthesis of various polycyclic ring systems. Probably the most important types of these polycyclic compounds are their fused heterocyclic and spiroheterocyclic representatives. Although such compounds have been known for decades, their syntheses have hitherto been scarcely reviewed [6,7]. For this reason, the major aim of our present review article is to compile the most important types of heterocyclic compounds synthesized by the reactions of selected groups of exocyclic α,β-unsaturated ketones, represented by 2-arylidene-1-indanones (1), 1-tetralones (2), 1-benzo-suberones (3), 3-arylidenechromanones (4), 1-thiochromanones (5), flavanones (6) and 1-thioflavanones (7).

2. Synthesis of Exocyclic α,β-Unsaturated Ketones

Several representatives of the above-mentioned exocyclic α,β-unsaturated ketones 1-7 have been well known compounds for a long time. 2-Arylidene-1-indanones (1), 1-tetralones (2) and 1-benzo-suberones (3) were synthesized by base- [8-20] and acid-catalyzed [21-26] condensation of 1-indanone, 1-tetralone and 1-benzo-suberone with aromatic aldehydes (Scheme 1). 3-Arylidenechromanones

Scheme 1

Scheme 2

Total Energy: 10.3313 Kcal / mol
Form compound H1

Total Energy: 23.5553 Kcal / mol
Form compound H6
Total Energy: 0.4658 Kcal / mol
Form compound H6

Total Energy: -30.1769 Kcal / mol
Form compound H9

Total Energy: -9.7397 Kcal / mol
Form compound H17

Total Energy: 7.2708 Kcal / mol
Form compound H17

Total Energy: 107.9837 Kcal / mol
Form compound H35

Total Energy: 33.3833 Kcal / mol
Form compound H35

Total Energy: 33.3833 Kcal / mol
Form compound H56
Total Energy: 8.6623 Kcal / mol
Form compound H57

Total Energy: 42.0151 Kcal / mol
Form compound H59

IR & UV of Compound 1,3-Di acetyl indol

IR & UV of Compound H54

IR & UV of Compound H1 Indol

NMR of Compound H2
References


