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SYNTHESIS AND CHARACTERIZATION OF A HETEROCYCLIC COMPOUND 5, 5, 8-TRIMETHYL HOMOCHROMAN

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ABSTRACT

Synthesis of 5, 5, 8-trimethyl homochroman was done by the reaction of m-cresol with 2-methyl 5-chloro pentene-2. The compound was found to be aromatic ether by elemental analysis and spectral data.

Key words: m-Cresol, Heterocyclic, Aromatic ether, IR, NMR, Homochroman, etc.

INTRODUCTION

A cyclic compound having at least two different atoms other than carbon i.e. N, O, S etc. as a member of ring are called heterocyclic compounds. 5, 5, 8-trimethyl homochroman is a seven member heterocyclic compound containing oxygen. It is confirmed as aromatic ether but not a phenolic compound by spectral analysis.

EXPERIMENTAL

Synthesis of 5, 5, 8-trimethyl homochroman (3)

15.78 g of 2-methyl 5-chloro pentene-2 and 7.35 g of m-cresol was mixed & heated at 140^{o}C for 12 hrs. HCl were released which was removed by aspiration after cooling. 200 mL of 20% aqueous KOH was used to dissolve the reaction mixture, followed by extraction with $C_2H_5COOCH_3$. Then drying over Na_2SO_4 and removal of the solvent from the neutral fraction was followed. The solid formed after drying was recrystallized from petroleum ether and pure 5, 5, 8-trimethyl homochroman was prepared.

During the heating of 2-methyl 5-chloro pentene-2 with m-cresol, two different products (1) & (2) were expected but none of them were produce.

The aromatic ether compound was indicated by IR bands with 1, 2-disubstituted benzene having a geminal dimethyl group. The NMR spectra were consistent with compound (3), showing spectrum of sharp singlet at δ 1.33 (6-CH_3 Protons) and a triplet at δ 3.4 (CH_3 adjacent to oxygen) as well as complex multiples δ 1.5 to 1.8 (4 aliphatic protons) and δ 6.8 to 7.7 (3 aromatic protons).

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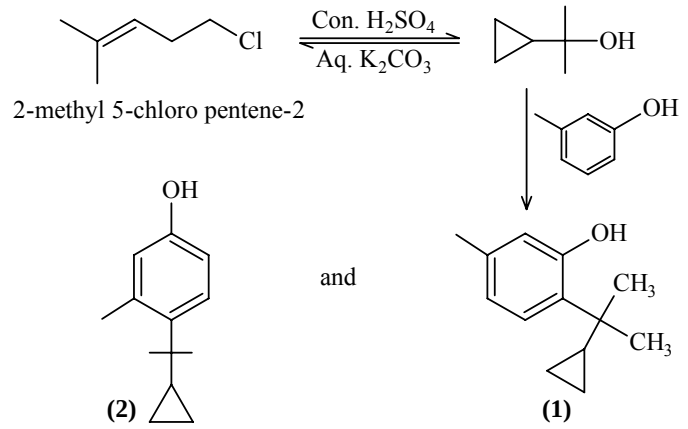
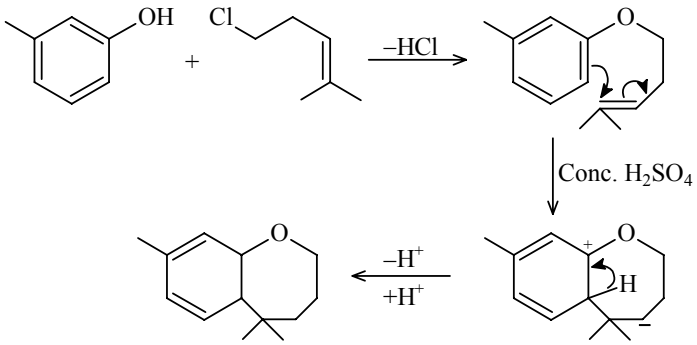


Neutral product formation

Neutral product (3) was formed first.

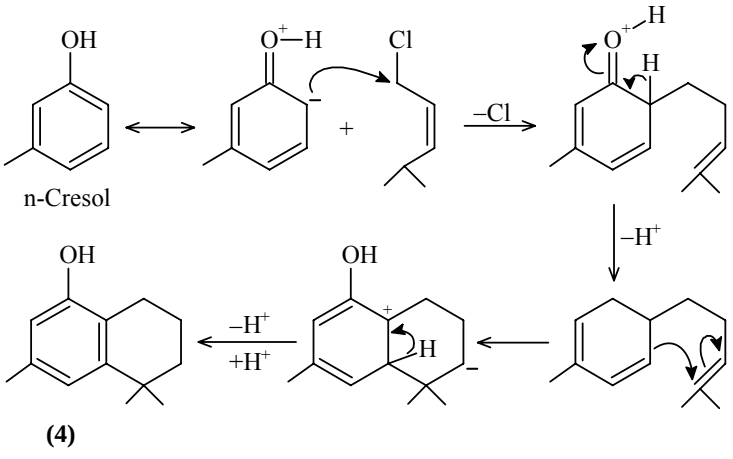


(3)

5,5,8-trimethyl homochroman

Phenolic product formation

Phenolic product (4) was formed next.



(4)

1,1,7-trimethyl 5-tetralol

Analytical data of compound (3)

Molecular formula: $C_{13}H_{18}O$, % of C = 82.10, % of H = 9.47, % of O = 8.42.

IR (KBr) in cm^{-1}: 1286 and 1226 (C-O-Ar stretching), 1382 and 1388 (CH_3-C-CH_3 stretching), 2845 and 2955 (Ar-CH_3 stretching).

NMR: 1.33 δ (6 H, Singlet) gem dimethyl group, 3.4 δ (2H, Triplet) CH_2-O α to Oxygen, 1.5 δ to 1.8 δ (4H, multiplets) two CH_2 groups, 6.8 δ to 7.7 δ (3H, multiplets) aromatic protons, 2.3 δ (3H, Singlet) Ar-CH_3.

Analytical data of compound (4)

Molecular formula: $C_{13}H_{18}O$, % of C = 82.10, % of H = 9.47, % of O = 8.42.

IR (KBr) cm^{-1}: 1380 and 1386 (CH_3-C-CH_3 stretching), 2845 and 2955 (Overlapping Ar-CH_3 stretching –CH_2-CH_2 stretching), 3550 (OH stretching).

NMR: 1.28δ (6 H, Singlet) gem dimethyl, 1.18 δ to 1.6 δ (4H, multiplets)methylenic proton, 2.57 δ (2H, Triplet) benzylic proton, 7.2 δ (3H, multiplets) aromatic protons, 2.4 δ (3H, Singlet) Ar-CH_3.

RESULTS AND DISCUSSION

The compound **(3)** is the oxygen containing seven member, heterocyclic, aromatic ether called as 5,5,8-trimethylhomochroman, which was confirmed by the elemental and spectral analysis.

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