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Research Article

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Synthesis and Identification of Oxygen containing seven membered Heterocyclic Compound 5,5,8-Trimethyl Homochroman

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ABSTRACT

5,5,8-trimethyl homochroman were synthesized by the reaction of m-cresol with 2-methyl 5-chloro pentene-2. Elemental analysis, IR and NMR suggested that it is an aromatic ether.

Keywords: Homochroman, m-cresol, Heterocyclic, Ether etc.

INTRODUCTION

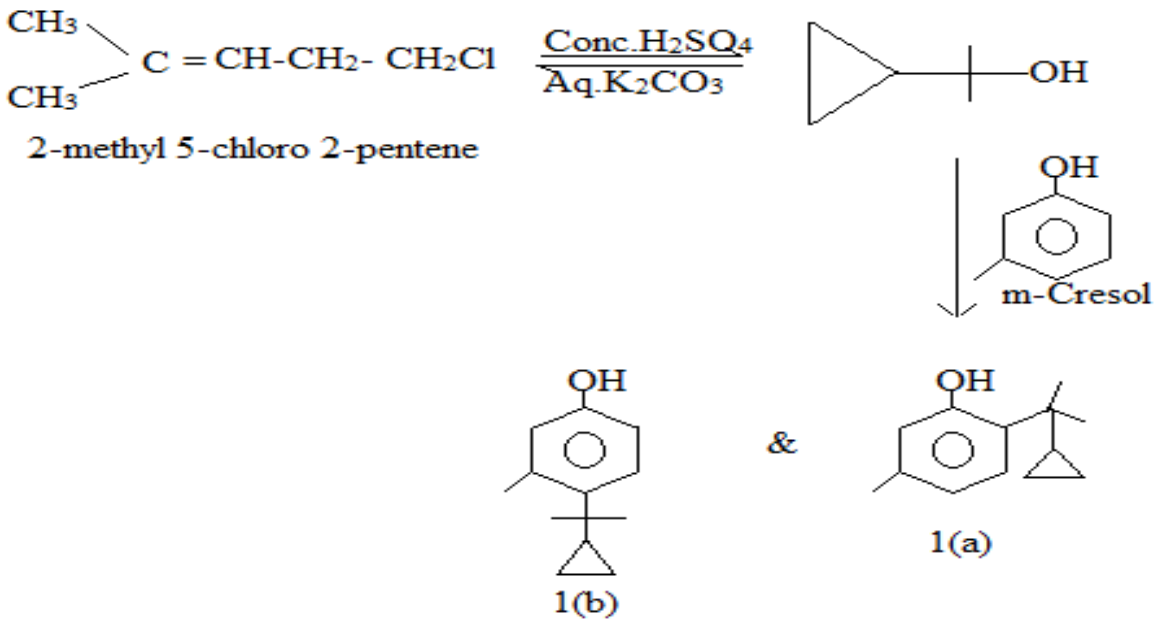
Heterocyclic compounds are cyclic compound of at least two different atoms (other than carbon i.e. N, O, S etc) as a member of ring. In recent past, heterocyclic compounds and chemistry has been very interesting part of the chemistry for their chemical and biological behavior. 5,5,8-trimethyl homochroman is seven membered oxygen containing heterocyclic compound. A slight change in the synthesis process of this compound leads to the formation of completely different product which is not a heterocyclic compound rather a phenolic compound.

EXPERIMENTAL SECTION

Chemicals used in the synthesis were of laboratory grade.

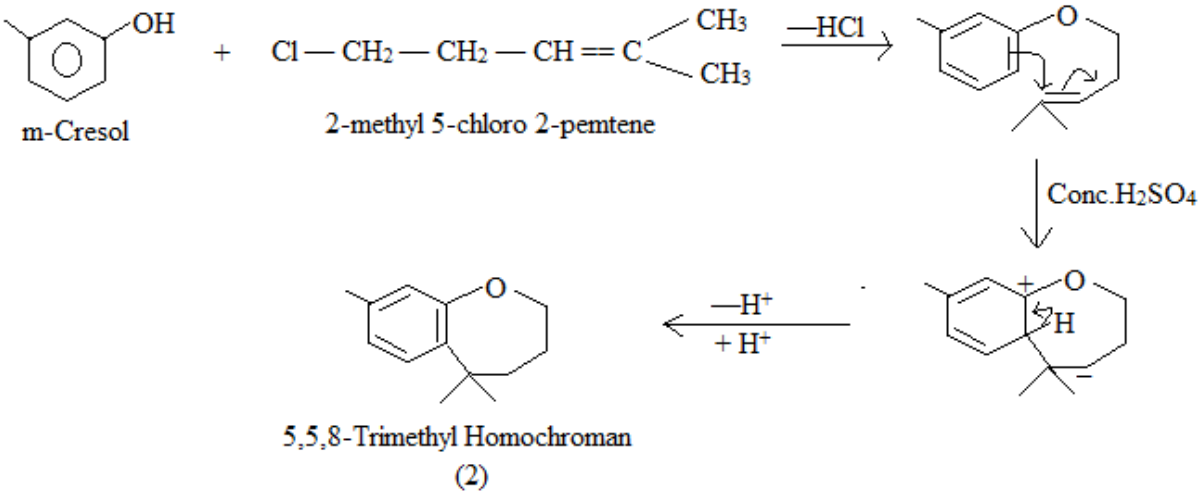
Synthesis of 5,5,8-trimethyl homochroman:
A mixture of 2-methyl 5-chloro 2-pemtene (15.78 gm) and m-cresol (7.35 gm) was heated at 140^{o}C for 12 hours, during which hydrochloride evolved. After cooling, the residual hydrogen chloride was removed by aspiration for several minutes. The reaction mixture was dissolved in 200 ml of 20% aqueous potassium hydroxide followed by extraction with ethyl acetate. After drying over sodium sulphate and removal of the solvent from the neutral fraction, a solid was obtained, which on crystallization from petroleum ether afforded pure 5,5,8-trimethyl homochroman (6.5 gm) and M.P. 48-50^{o}C.

When 2-methyl 5-chloro 2-pemtene were heated with m-cresol, 1(a) & 1(b) were the expected product.

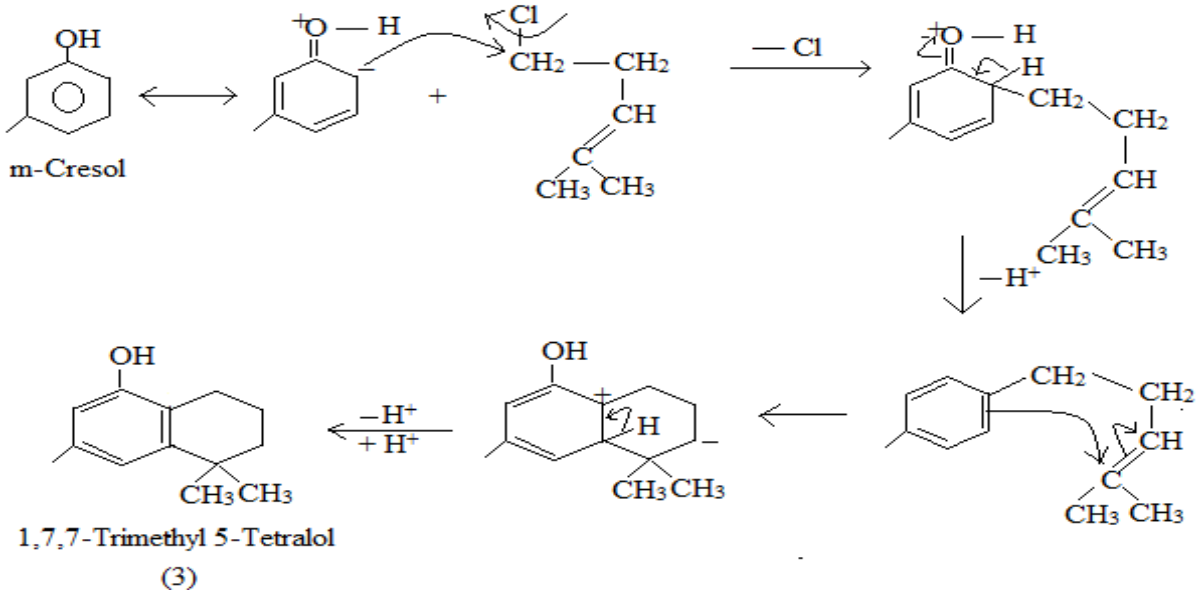


But in actual observed course of reaction, two products were obtained and surprisingly none of these was 1(a) & 1(b).

Formation of Neutral product:
The following reaction sequence leading to the formation of neutral product (2).



Formation of Phenolic product:
The following reaction sequence leading to the formation of phenolic product (3).



Identification of 5,5,8-trimethyl homochroman was based upon the spectral data. Infra red bands indicated that the compound was an aromatic ether, a 1,2-disubstituted benzene and had a gem dimethyl group. The NMR spectra was consistent with compound (2). The spectrum had a sharp singlet at δ 1.33 (six methyl protons) and a triplet at δ 3.4 (methyl adjacent to oxygen) as well as complex multiplets δ 1.5 to 1.8 (four aliphatic protons) and δ 6.8 to 7.7 (three aromatic protons).

Data for compound (2):

Molecular Formula : $C_{13}H_{18}O$
C : 82.10%
H : 9.47%
O : 8.42%

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

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

Data for compound (3):

Molecular Formula : $C_{13}H_{18}O$
C : 82.10%
H : 9.47%
O : 8.42%

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

NMR:
δ 1.28 (6 H, Singlet) for gem dimethyl
δ 1.18 to 1.6 (4H, multiplets) for methylenic proton

δ 2.57 (2H, Triplet) for benzylic proton
δ 7.2 (2H, multiplets) for aromatic protons
δ 2.4 (3H, Singlet) for Ar-CH_3.

RESULTS AND DISCUSSION

The elemental analysis and spectral data support the compound (2) as an official compound i.e. 5,5,8-trimethyl homochroman, an aromatic ether.

REFERENCES

[1] Asif Hussain and Priyanka Ahuja, *Acta Poloniae Pharm*., **2008**,65, 527.
[2] R. Franski, *Aaian J.Chem*., **2005,** 17, 2063.
[3] Y. J. Bian, J. T. Li and T. S, Li, *Chin J. Org Chem*.,**2007,** 22, 227.
[4] N. M. M. Benzerra, S. P. Oliveria and R. M. Srivastava, *Farmaco*., **2005**, 60, 955.
[5] Sajeevan Gaikwad, Venkat Suryawanshi, Yogiraj Vijapure and Vishnu Shinde, *J. Chem. Pharm. Res.,* **2012**, 4(3),1851-1855
[6] J. Rajora, J. Yadav, R. Kumar, and Y. K. Srivastava. *Indian Journal of Chemistry.,* **2010,** 49B, 989.
[7] H. S. Schaff and A. I. Zumla. *JAMA*., **2009,** 302, 2488.
[8] E. Gursoy, N. Guzeldemirci Ulusoy, *Eur.J.Med.Chem.*, **2007,** 42, 320.
[9] R. Kalsi, M. Shrimali,T. N. Bhalla, J. P. Barthwal, *Indian J.Pharm.Sci*., **2006**, 41, 353.
[10] Nitesh Chauhan, Kartik Vyas, Kiran Nimavat, Kaushik Joshi, *J. Chem. Pharm. Res.,* **2012**, 4(2), 1106-1110
[11] H. S. Patel,V. K. Patel. *Ind. J. Heterocyclic Chem*., **2003**, 12, 253.
[12] V. V. Mulwad, B. P. Choudhari. *Ind.J.Heterocyclic Chem., **2003,** 12, 197*.
[13] Sambhaji P. Vartale, Nagesh D. Kalyankar, Nilesh K. Halikar, *J. Chem. Pharm. Res.*, **2012**, 4(1), 186-191
[14] M. Gupta, B. S. Bairwa, R. Karan, I. K. Sharma and P. S. Verma. *Indian J.Chem*., **2008,** 47A, 383.
[15] C. Sowjanya, V. RamaBharathi, G. Kalpana Devi and G. Rajitha, *J. Chem. Pharm. Res.*, **2011**, 3(6), 212-216.