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SYNTHESIS OF SOME NOVEL OXAZEPINES FROM SCHIFF BASES

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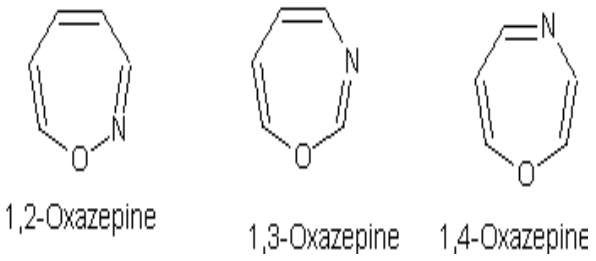
ABSTRACT
The oxazepine compounds are synthesized by condensation reaction of Schiff base with phthalic, maleic and succinic anhydride. The structure of synthesized oxazepines were characterized by FTIR method and melting point determination.

KEYWORDS: Schiff base, 2-hydroxy-5-methylacetophenone, Oxazepine, FT-IR spectra.

INTRODUCTION

Oxazepines are 7-membered heterocyclic compounds containing nitrogen and oxygen heteroatoms.[1] These compounds have been synthesized by condensation of Schiff bases and anhydrides.[2] The oxazepine compounds are classified according to the position of heteroatom such as 1,2-oxazepine,1,3-oxazepine and 1,4oxazepine.



The 1,3 and 1,4-oxazepines are important and have wide biological activities and pharmaceutical applications such as antibacterial , antidepressant, antiviral, antitumor and anti-inflammatory herbicides, pesticides, lubricants and analytical reagents.[3-6]

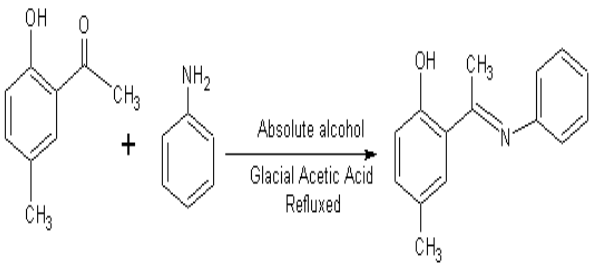
The Schiff bases are important intermediates and precursor for the synthesis of oxazepine derivatives and contain-C=N group.[7] The Schiff bases can be synthesized by condensation of an amine and active carbonyl group like aldehyde and ketone which shows various biological activities.[8-10]

In this study some novel Schiff bases have been synthesized from 2-hydroxy-5-methyl acetophenone and aniline and then oxazepine compounds were synthesized by condensation of Schiff base and anhydride.

METHODS AND MATERIALS

Synthesis of Schiff base (I)

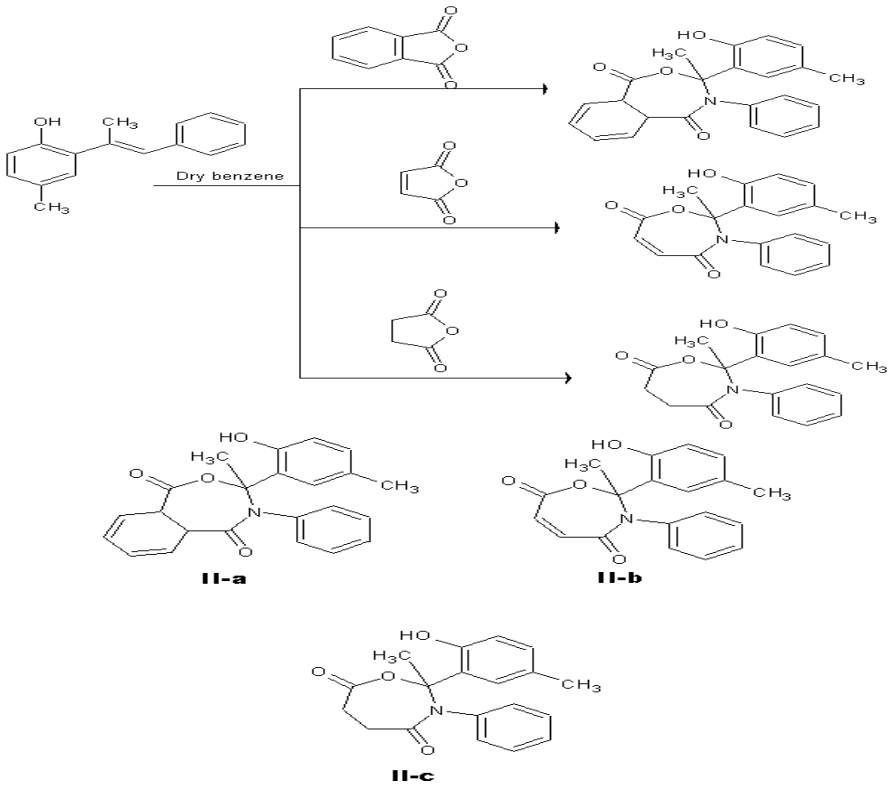
2-Hydroxy-5-methyl acetophenone (1.95gm, 0.013mol) was dissolved in 15 ml absolute ethanol containing two drops of glacial acetic acid, then equimolar amount of aniline (1.18gm,0.013mol) was added. The reaction mixture refluxed with stirring for 4hr. Then the mixture was evaporated. The colored precipitate was filtered and washed with cold ethanol.**m.p.-45°C.**



Compound-I

Synthesis of Oxazepine compounds(II-a, II-b, II-c)

A mixture of Schiff base (0.007mol) and anhydride (0.007mol) were grinded with mortar, mixed, dried and dissolved in dry benzene. The reaction mixture was refluxed with stirring at 85°C for 5 hours. The mixture was then allowed to cool at room temperature, a coloured precipitate of oxazepine was obtained, which was filtered and re-crystallized from dioxane.[1]



RESULT AND DISCUSSION

The melting points of synthesized compounds were sharp. The compounds were characterized by FT-IR spectra.

IR spectra of N-[(2-hydroxy-5-methylphenyl)ethylidene]-1-aniline (Schiff base(I)

The band at 1629cm^{-1} due to *v*(-C=N) group, 1490cm^{-1} due to the v(C=C) of aromatic benzene ring, 2924cm^{-1} due to the v(C-H), 1244cm^{-1} due to *v*(C-H) of aromatic benzene in plane bending, 1209cm^{-1} due to *v* (-C-O) of phenol, 964,881 and 783cm^{-1} due to the *v*(C-H) of aromatic benzene out of plane bending. **M.P:-45^{o}C.**

IR spectra of 2-[2-hydroxy-5-methylphenyl]-2-methyl-3-phenyl-2,3-dihydro-5,6-benz-[1,3]-oxazepine-4,7-dione(II-a)

The presence of two strong absorption bands at 1710cm^{-1} for lactone and 1589cm^{-1} for lactum. The other absorption bands are 2924cm^{-1},3026 and 3072cm^{-1} due to *v*(-C-H) of aromatic benzene ring, 1944,1462 and 1390cm^{-1} due to *v*(-C=C-) of aromatic benzene ring, 1629cm^{-1} due to *v*(-C=N), 1219cm^{-1} due to *v*(C-O) of phenol, 1120 and 1072cm^{-1} due to *v*(-C-O-C-) and *v*(-C-N-C) respectively. **M.P:-135^{o}C**

IR spectra of 2-[2-hydroxy-5-methylphenyl]-2-methyl-3-phenyl-2,3-dihydro-[1,3]-oxazepine-4,7 dione(II-b)

The bands at 1709cm^{-1} for lactone and 1634cm^{-1} for lactum, 3010, 2924cm^{-1} due to *v*(-C-H), 1629cm^{-1} due to *v*(-C=N), 1487,1435,1365cm^{-1} due to *v*(C=C) of aromatic benzene ring, 1242cm^{-1} due to *v*(C-O) of phenol, 1159 and 1020cm^{-1} due to *v*(-C-O-C-) and *v*(-C-N-C) respectively. **M.P:-220^{o}C**

IR spectra of 2-[2-hydroxy-5-methylphenyl]-2-methyl-3-phenyl-2,3,5,6-tetrahydro-1,3-oxazepine-4,7-dione(II-c) The bands at 1701cm^{-1} for lactone and 1543cm^{-1} for lactum, 1624cm^{-1} due to *v*(C=N),2990-3099cm^{-1} due to *v*(-C-H), 1496,1410,1370cm^{-1} due to *v*(C=C) of aromatic benzene ring, 1219cm^{-1} due to *v*(C-O) of phenol. **M.P:-40^{o}C.**

Ring strain in cyclic compounds causes a complementary large shift of the C=O stretching to a higher frequency, this provides a dependable test to distinguish clearly between three, four, five and larger membered ring ketones. The same effect is observed with cyclic ester which are called lactones and cyclic amides which are called lactumes. In fact carbonyl stretching frequency reaches its maximum in highly strained β-lactume(1800cm^{-1}).When lactum ring is fused to another ring a general increase in the C=O stretching frequency to the extent of 20-50cm^{-1} is observed.

CONCLUSION

The present study reveals that all the three synthesized oxazepine compounds shown good agreement with IR spectral data. Study of literature survey also conclude that these oxazepines may possess some biological activities.

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