Synthesis and Biological Evaluation of Some Ethers Acetylene Compounds Derivatives of Oxazole

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Abstract

In this present synthesis anew series of some ethers acetylene compounds derivatives of

2-p-hydroxy benzyl-4,5-ditolune oxazole.

2-p-hydroxy benzyl-4-tolune-5-phenyl oxazole.

2-p-hydroxy benzyl-4,5-di-p-chloro phenyl oxazole.

2-p-hydroxy benzyl-4,5-di-p-bromo phenyl oxazole.

2-p-hydroxy benzyl-4-p-dimethyl amino phenyl -5-phenyl oxazole.

Treated with 3-bromo propyne yielded series of new ethers acetylene oxazole compounds were characterized by (FT-IR , 1HNMR , 13CNMR , C.H.N) in this study of the effect compound in the two types of bacteria isolated from amedical condition (human) .

Keywords: *OXAZOLE, 3-Bromo Propyne, Benzoine.*

INTRODUCTION

The oxazole moieties have abroad spectrum of biological activity compounds including antiarrhythmics (1) , anticonvulsant (2) , anti bac- -teria (3) and antifungal .

In addition to it's connection acetylene group increased importa- -nce biological ethers acetylene importance of pharmaceutical (5,6,7,8) and drugs used to parkinson's disease (9, 10). Such as inhibiting drugs to work acetylcholine.

The new derivatives were in characterized on the (FT-IR , 1HNMR , 13CNMR , C.H.N) another study includes the biological activity .

Unless otherwise stated the following generalization melting point (FT-IR , 1HNMR , 13CNMR , C.H.N)

1. Synthesis of oxazole (11 ,12) :

Symmetrical benzoin or unsymmetrical (0.01 mol) were treated with α-amino acid tyrosine (0.01 mol) homogeneous mixture

and heated on an oil bath until the release of carbon dioxide and ammonia

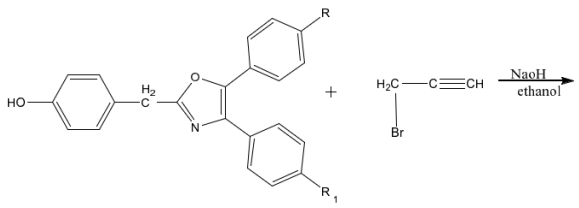
Then we add ethanol refluxed (15 min) . The solution was then cold (24 hr) and crystallization by ethanol.

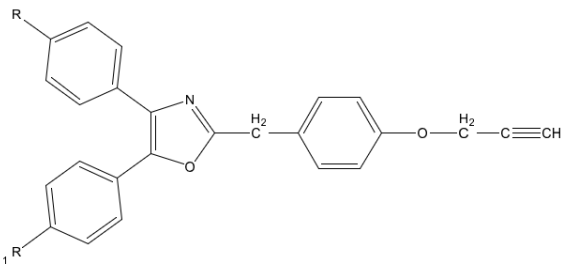
2. Synthesis of acetylene ethers compounds (13 , 14) :

Dissolved (0.01 mol) oxazole in (5 gm) NaOH and (50 ml) ethanol and stirred for (15 min) then added drop-wise to the well stirred reaction mixture the which was heated to (60 – 70 c◦) to (3 hr) , The reaction was stopped and the mixture was cooled to room temperature. An Ice water was added to the reaction mixture and the crude product was extracted twice by ethylene chloride and crystalaztion by ethanol.

Results and Discussion

The synthesis of acetylene compounds by reaction oxazole with 3-bromo propyne yielded new compounds:





R1 = CH3, CL, Br, N(CCH3)2

R2 = H, CH3, CL, Br

SCHEME:

The mechanism of preparing acetylene compound

The reaction was concluded to occoure via SN2 mechanism terminal alkyne was prepared by condensing oxazole with propargyl bromide in dilute ethanolic sodium hydroxide solution at (70 c◦) according to nuchlophilic substitution reaction .

The acetylene compound were characterized using (M.P) and (C.H.N) anlysis (Table 1) , and (FT-IR , 1HNMR , 13CNMR) anlysis (Table 2,3,4) and Antic bacterial activity (Table 5).

The newly acetylene compound disappearance spectral (OH) in oxazole at (3500 cm-1), appearance of acetylene group in (2200 cm-1) The ether acetylene very important the biological activity:

Table (1) : Analytical data of acetylene compound

Com .No	Molecular Formule	M.wt g/mol	Color	Yield%	M.P.C	C%	H %	N%
1	C27H23NO2	393.276	Light yellow	66%	93-97	82.454 82.472	5.848 5.455	3.561 3.577
2	C27H23N2O2CL	442.735	Brown	63%	63-69	73.242 73.231	5.195 5.133	6.327 6.345

3	C25H17NO2CL2	434.162	yellow	71%	94-96	69.156 69.119	3.915 3.973	3.225 3.238
4	C25H17NO2Br2	523.256	Light yellow	60%	73-76	57.381 57.366	3.248 3.256	2.676 2.653
5	C27H24N2O2	408.282	auburn	70%	Oily	79.423 79.459	5.878 5.867	6.860 6.876
6	C26H21NO2	379.266	Brown	68%	92-95	82.332 82.376	5.537 5.582	3.692 3.633

Table (2): FT-IR of acetylene compounds

$C_{27}H_{23}NO_2$ (cm^{-1})	C=C(1622),C-C(1100),C-O(1224), C-N(1020),C-H(2900),=C-H(3100), C≡C(2200), ≡C-H(3300)
$C_{27}H_{23}N_2O_2CL$ (cm^{-1})	C=C(1650),C-C(1150),C-O(1200), C-Cl(850),C-N(1230),C-H(2950), =C-H(3125),C≡C(2260), ≡C-H(3200)
$C_{25}H_{17}NO_2CL_2$ (cm^{-1})	C=C(1620),C-C(1300),C-O(1050), C-CL(877),C-N(1200),C-H(2950), =C-H(3100),C≡C(2200), ≡C-H(3300)
$C_{25}H_{17}NO_2Br_2$ (cm^{-1})	C=C(1620),C-C(1100),C-O(1225), C-Br(690),C-N(1210),C-H(2900), =C-H(3100),≡C C(2200), ≡C-H(3300)
$C_{27}H_{24}N_2O_2$ (cm^{-1})	C=C(1622),C-C(1100),C-O(1224), C-N(1200),C-H(2900),=C-H(3100), C≡C(2200), ≡C-H(3300)
$C_{26}H_{21}NO_2$ (cm^{-1})	C=C(1620),C-C(1100),C-O(1220), C-N(1200),C-H(2900),=C-H(3100), C≡C(2200), ≡C-H(3300)

Table (3): HNMR of compounds

C27H23NO2	≡C-H(2.5ppm)(1H,S), O-CH_2(3.4ppm)(2H,S), CH_2(1.3ppm)(2H,D),Ph(7.2ppm)(4H,D), CH_3(2.4ppm)(3H,S)
C27H23N2O2Cl	≡C-H(2.3ppm)(1H,S), O-CH_2(3.5ppm)(2H,S), CH_2(1.1ppm)(2H,D),Ph(7.4ppm)(4H,D), CH_3(2.5ppm)(3H,S),N-CH_3(0.9ppm)(3H,S)
C25H17NO2Cl2	≡C-H(2.4ppm)(1H,S), O-CH_2(3.2ppm)(2H,S), CH_2(1.3ppm)(2H,D),Ph(7.1ppm)(4H,D), CH_3(2.2ppm)(3H,S)

C25H17NO2Br2	**≡C-H(2.5ppm)(1H,S), O-CH_2(3.6ppm)(2H,S), CH_2(1.4ppm)(2H,D),Ph(7.6ppm)(4H,D), CH_3(2.4ppm)(3H,S)**
C27H24N2O2	**≡C-H(2.5ppm)(1H,S), O-CH_2(3.5ppm)(2H,S), CH_2(1.4ppm)(2H,D),Ph(7.3ppm)(4H,D), CH_3(2.5ppm)(3H,S),N-CH_3(0.9ppm)(3H,S) Ph(7.8ppm)(5H,T)**
C26H21NO2	**≡C-H(2.5ppm)(1H,S), O-CH_2(3.1ppm)(2H,S), CH_2(1.2ppm)(2H,D),Ph(7.2ppm)(4H,D), CH_3(2.5ppm)(3H,S),N-CH_3(0.9ppm)(3H,S) Ph(7.6ppm)(5H,T)**

Table (4): CNMR of Compounds

C27H23NO2	**C≡C(72ppm),C=C(123ppm) ,Ph(162ppm), CH_3(22ppm), C-N(57ppm),C=N(157ppm), C-O(74ppm).**
C25H17NO2Cl2	**C≡C(72ppm),C=C(122ppm), Ph(160ppm), CH_3(17ppm), C-N(44ppm),C=N(153ppm), C-O(63ppm),C-Cl(77ppm).**
C25H17NO2Br2	**C≡C(80ppm),C=C(142ppm), Ph(138ppm), CH_3(26ppm), C-N(42ppm),C=N(157ppm), C-O(67ppm),C-Br(59ppm).**
C27H24N2O2	**C≡C(84ppm),C=C(138ppm), Ph(118ppm), CH_3(32ppm), C-N(51ppm),C=N(145ppm), C-O(68ppm).**
C26H21NO2	**C≡C(70ppm),C=C(131ppm), Ph(133ppm), CH_3(26ppm), C-N(48ppm),C=N(146ppm), C-O(71ppm).**

Table (5): Biological activity of new ethers acetylene compounds

Com .No	Staphylococcus aureus	Escherichia Coli
1	**+++**	**+**
2	**+++**	**-**
3	**++**	**++**
4	**+++**	**-**
5	**+**	**++**
6	**++**	**-**

. 11-5= +++ (highly active)

. 0-10= ++ (active)

. 1-5 = + (slightly active)

The results of anti bacterials were present in table (5) in this study of the effect of bacteria isolated from amedical condition(human) and it Has studied and diagnosed and proved their attributes .

CONCLUSION:

In conclusion a series of symmetrical and unsymmetrical oxazole With propargyl bromide give new ethers acetylene compounds the reaction good yield and products in future .

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