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MASS SPECTROMETRY OF SOME NEW 2-HYDROXYMETHYL-5-PHENYL-FURANS OBTAINED THROUGH CELL CATALYSIS

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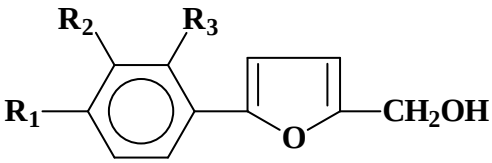
ABSTRACT. Eight 2-hydroxymethyl-5-phenyl-furans were obteined from the corresponding aldehydes through reaction with *Saccharomyces cerevisiae*. The fragmentation scheme showed the M^+ - 17 peaks for every system studied and characteristic features for the heterocyclic moiety of the alcohols. Some details are discussed within the fragmentation scheme for each compounds.

INTRODUCTION

As a part of our researches in the furan series we have prepared eight new from the corresponding aldehydes using Sacharomices cerevisiae as reducting agent [6].



a: R_1 = F; R_2 = H; R_3 = H
b: R_1 = Cl; R_2 = H; R_3 = H
c: R_1 = Br; R_2 = H; R_3 = H
d: R_1 = I; R_2 = H; R_3 = H
e: R_1 = H; R_2 = Br; R_3 = H
f: R_1 = H; R_2 = H; R_3 = Cl
g: R_1 = H; R_2 = H; R_3 = Br
h: R_1 = H; R_2 = H; R_3 = I

Scheme 1

This paper deals with the mass spectra of these compounds. We considered it of interest to find out to what extent the characteristic fragmentation modes of furans[1-5], are also presents in the case of a-h and what is the influence of the hydroximethyl group in position 2 on the furan ring upon the fragmentation process.
Mass spectral data m/e (I%):

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a: 51(10,6), 57(8,6), 75(15,5), 83(9,6), 91(10,5), 95(19,5), 107(10,8), 109(10,8), 118(11,3),120(6,4), 123(34,8), 133(48,3), 134(11,2), 135(10,1), 145(12,7), 146(23,7), 147(19,6), 163(9,1), 164(8,7), 175(99), 176(13), 187(3), 188(7,3), 192(100), 191(13)
b: 29(13,4), 39(12), 46(21,3), 63(31,4), 75(41,3), 87(26,3), 91(11), 111(33), 112(6), 113(16,7), 114(19,8), 115(41,6), 116(22,2), 117(11,6), 127(33,8), 128(41,6), 139(39,7), 140(9,1), 141(9,3), 142(3), 149(43,6), 150(6,3), 151(22,8), 161(2), 162(8,3), 163(7,1), 164(5), 165(4), 178(6), 179(8), 180(10,1), 181(6,3), 182(4,1), 191(74,5), 192(13,6), 193(26,3), 194(5,1), 205(10,1), 206(23,1), 208(100), 209(25,3), 210(33,5), 211(6,1)
c: 29(10), 50(11), 63(18,2), 78(13), 88(16), 91(13), 109(33), 110(43,6), 111(43,6), 112(43,6),113(53), 114(41,6), 115(21,6), 127(30), 128(57,2), 129(59,6), 144(27), 145(13),155(14),157(14), 183(32),185(32),193(12),195(12),224(13), 226(13),235(62), 236(20), 236(62), 237(20), 250(8), 251(13,6), 252(100), 253(31,3), 254(100), 255(10)
d: 63(3), 74(2), 88(4), 91(11,2), 115(13), 135(6,3), 149(2), 171(2,6), 203(6,3), 241(21), 270(6), 283(81), 298(60), 299(30), 300(100), 301(10)
e: 29(10), 50(11), 63(18,2), 78(13), 88(16), 91(13), 109(33), 110(43,6), 111(43,6), 112(43,6),113(53), 114(41,6), 115(21,6), 127(30), 128(57,2), 129(59,6), 144(27), 145(13), 155(14),157(14), 183(32), 185(32), 193(12), 195(12), 224(13), 226(13), 235(62),236(20), 236(62),237(20), 250(8), 251(13,6), 252(100), 253(31,3), 254(100), 255(10)
f: 29(13,4), 39(12), 46(21,3), 63(31,4), 75(41,3), 87(26,3), 91(11), 111(33), 112(6), 113(16,7), 114(19,8), 115(41,6), 116(22,2), 117(11,6), 127(33,8), 128(41,6), 139(39,7), 140(9,1), 141(9,3), 142(3), 149(43,6), 150(6,3), 151(22,8), 161(2), 162(8,3), 163(7,1), 164(5), 165(4), 178(6), 179(8), 180(10,1), 181(6,3), 182(4,1), 191(74,5), 192(13,6), 193(26,3), 194(5,1), 205(10,1), 206(23,1), 208(100), 209(25,3), 210(33,5), 211(6,1)
g: 29(10), 50(11), 63(18,2), 78(13), 88(16), 91(13), 109(33), 110(43,6), 111(43,6), 112(43,6),113(53), 114(41,6), 115(21,6), 127(30), 128(57,2), 129(59,6), 144(27), 145(13), 155(14),157(14), 183(32), 185(32), 193(12), 195(12), 224(13), 226(13), 235(62), 236(20), 236(62),237(20), 250(8), 251(13,6), 252(100), 253(31,3), 254(100), 255(10)
h: 63(3), 74(2), 88(4), 91(11,2), 115(13), 135(6,3), 149(2), 171(2,6), 203(6,3), 241(21), 270(6), 283(81), 298(60), 299(30), 300(100), 301(10)

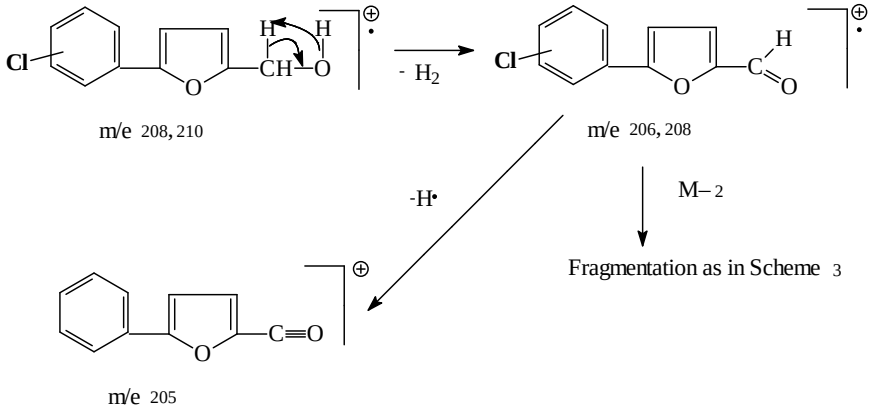
RESULTS AND DISCUSSION

In order to simplify the interpretation of the mass spectra of our compounds we recorded also the spectrum of 5-phenyl-furyl-2-carboxaldehydes substituted with halogenes at the phenylic ring as model.

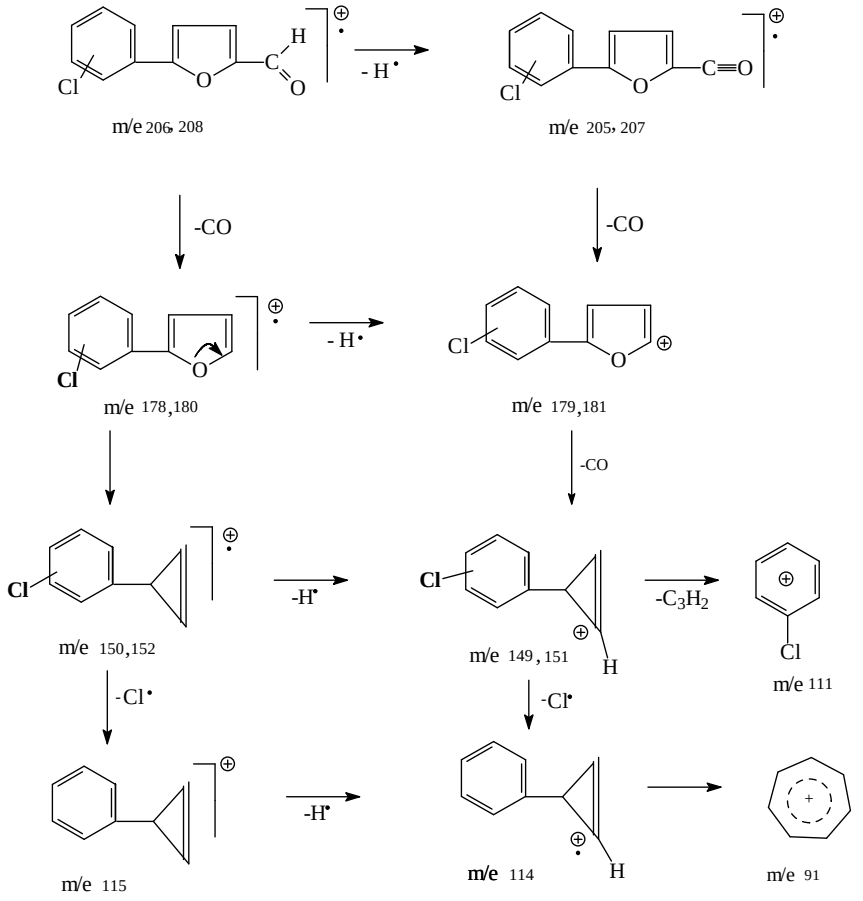
In case of bioproducts we observed a fragmentation characteristic for benzylic alcohols. The molecular ion is the base peak M - 1, M - 2, M - 3 are observed too. Slow intensity M+1 peak is appeared.

For exemplification we presented the fragmentation mode of chloroderivatives.

The fragments presents in Scheme 3 are also appeared in the mass spectras of the corresponding aldehydes too.

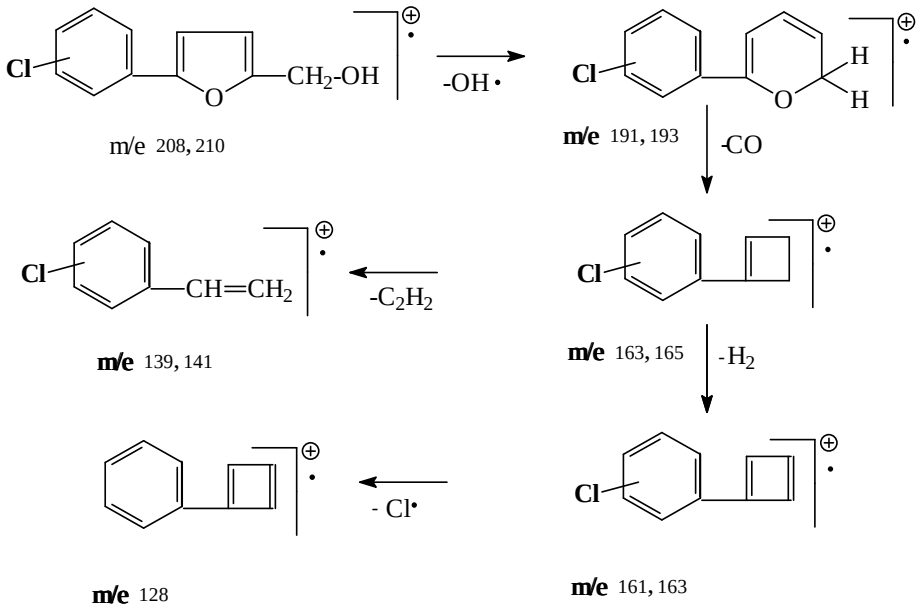


Scheme 2



Scheme 3

An other way for the cleavage presented in Scheme 4 is with elimination of an -OH radical. We supposed that the M - 17 sufered a ring rearrangement which cleaves with elimination of -CO and gives a cyclobutadienylic ring as in case of hydroxymethyl-furyl benzothiazoles [7].



Scheme 4

Each substances presents the same pattern of the fragmentation. In case of c, e, g its observed the presence of two bromine isotope (79,81).

The substance presents two molecular peaks (M= 252, 254) with the same abundance and two characteristic fragments for the benzylic alcohols, M-17 (225, 227). For substances b and f the two chloro isotope (35, 37) are present, two molecular peaks (208, 210) and two characteristic fragments, M-17 (191, 193) are appeared.

Molecular peaks for (a-h) are clear with an relative abundance of 100%.

EXPERIMENTAL

The purity of the substances was checked by TLC on silica gel. The mass spectra were recorded using a Double focusing VARIAN MATT 311 Spectrometer with an electronic impact at 70 eV and 300 mA. The source temperature was 150-200^{0}C.

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