

MASS SPECTRA OF SOME 2,6 - DIARYL - 4 - PYRIDONES AND THEIR THIO ANALOGUES

Mohamed Gaber Marei

Chemistry Department, Faculty of Science, Alexandria University

Ibrahimia P.O. Box 426, Alexandria, Egypt

ABSTRACT

The mass Spectra of 2 - P - chlorophenyl - 1 - methyl - 6 - Phenyl-4 - Pyridone 1, 2,6 - diphenyl-1 methyl-4 - thiopyridone 2, 2 - P - bromophenyl - 1 - methyl-6 - phenyl-4 - Pyridone sulfone - 1 - oxide³ and 3,5 - dibromo - 2,6 - diphenyl-1 - methyl-4 - pyridone sulfone - 1 - oxide⁴ are reported and discussed . The spectra of these compounds are different from the parent 4 - pyridone . The retro Diels - Alder reaction is observed in their spectra . Loss of CX from the molecular ion competes favorably with retro Diels - Alder reaction .

INTRODUCTION AND DISCUSSION

The chemistry of 2,6- diaryl - 1 methyl - 4 - pyridones, thiopyridones and sulfone - 1 - oxides previously has been investigated in this laboratory, owing to their interesting properties both in fundamental, synthetic or biological fields 1,2 . These pyridones and thiopyridones are usually obtained by reaction of the respective 4 - pyridones and thiopyridones with methylamine 1,3,4. while 4 - pyridone sulfone - 1 - oxides are formed by action of hydrogen peroxide on 4 - thiopyridones³. This paper deals with a study of the frag-

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mentation patterns of the title compounds by electron impact mass spectrometry .

while the mass spectra of 4 - pyridone⁵ and 2 - phenyl - 6 - methyl - 4 - pyridone⁶ have been reported, information is lacking in the literature, however, on the mass spectral fragmentation of 2,6 - diaryl - 1 - methyl - 4 pyridones and their sulfur analogs .

In the present study, I will discuss the electron impact mass spectrometry of compounds 1 - 4 with a two - fold aim : i) to describe the most important fragmentation pathways ' ii) to study, via mass spectrometric technique, the effect of substituents on the intensity of fragments and pathways. It is observed that the mass spectrum of 2,6 - diphenyl - methyl - 4 - thiopyridone 2 gave the molecular ion as the base peak, while 2 - p - chlorophenyl - 1 - methyl - 6 - phenyl - 4 - pyridone 1 showed low intense molecular ion peak. however, the mass spectrum of 4 gave no molecular ion peak, this may be due to the ease of elimination of the bromine molecule¹ (Scheme, Table).

Table: Relative Intensity (%) of the Significant peaks in the Mass Spectra of the Compounds.1-4

Compd	Relative intensity (%) of				
	M ⁺	i	ii	iii	iv or v
1	4, 13	40	9, 25	14, 43	5, 9
2	100	13	13	58	13
3	6, 6	12		10	10, 9
4		7	5	12	4

The interesting fragmentation process in the spectra of compounds 1 - 4 was the retro Diels - Alder reaction, which gave rise to the species i and ii . However, the ketene species expected to be formed in these reactions were not observed : a behaviour reported for 2,6 - diaryl - 4H - pyran - 4 - ones⁷ . It is worth noting that the parent 4 - pyridone does not lose the elements of acetylene in a retro Diels - Alder reaction⁵ .

Similar to the parent 4 - pyridones⁵, the important fragmentation process was the expulsion of CX leading to the pyrrole species iii which showed the azafulvene cation iv or perhaps the ring - expanded species v by loss of hydrogen or OH radical . The formation of the species iv or v is usually observed in the spectra of N - methylpyrroles as the chief feature⁸ . Moreover, the species iii gave rise to a series of fragments characteristic of N - methylpyrroles⁸ .

EXPERIMENTAL

Mass spectra were measured with a Hitachi perkin - Elmer RMU6D double - focusing mass spectrometer, with an inlet and source temperature of approximately 150 °C. Spectra were measured at 70 eV

The pyridone derivatives 1- 3 were prepared as previously described^{1,3} . Purity was assessed by IR, ¹Hnmr , thin layer Chromatography and combustion analysis .

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Compound 4 was prepared (90 % yield) from 2,6 - diphenyl-1-methyl - 4 - Pyridone Sulfone - 1 - oxide and bromine in glacial acetic acid as described earlier³. This Product was crystallized from methanol in needles, m. p. 230⁰; IR : γ_{\max} (cm⁻¹) 1260 (NO); ¹H nmr :

(DMSO- d₆), δ / ppm) 3. 76 (s, N-CH₃). 7.78 - 7. 90 (m, Ar-H).

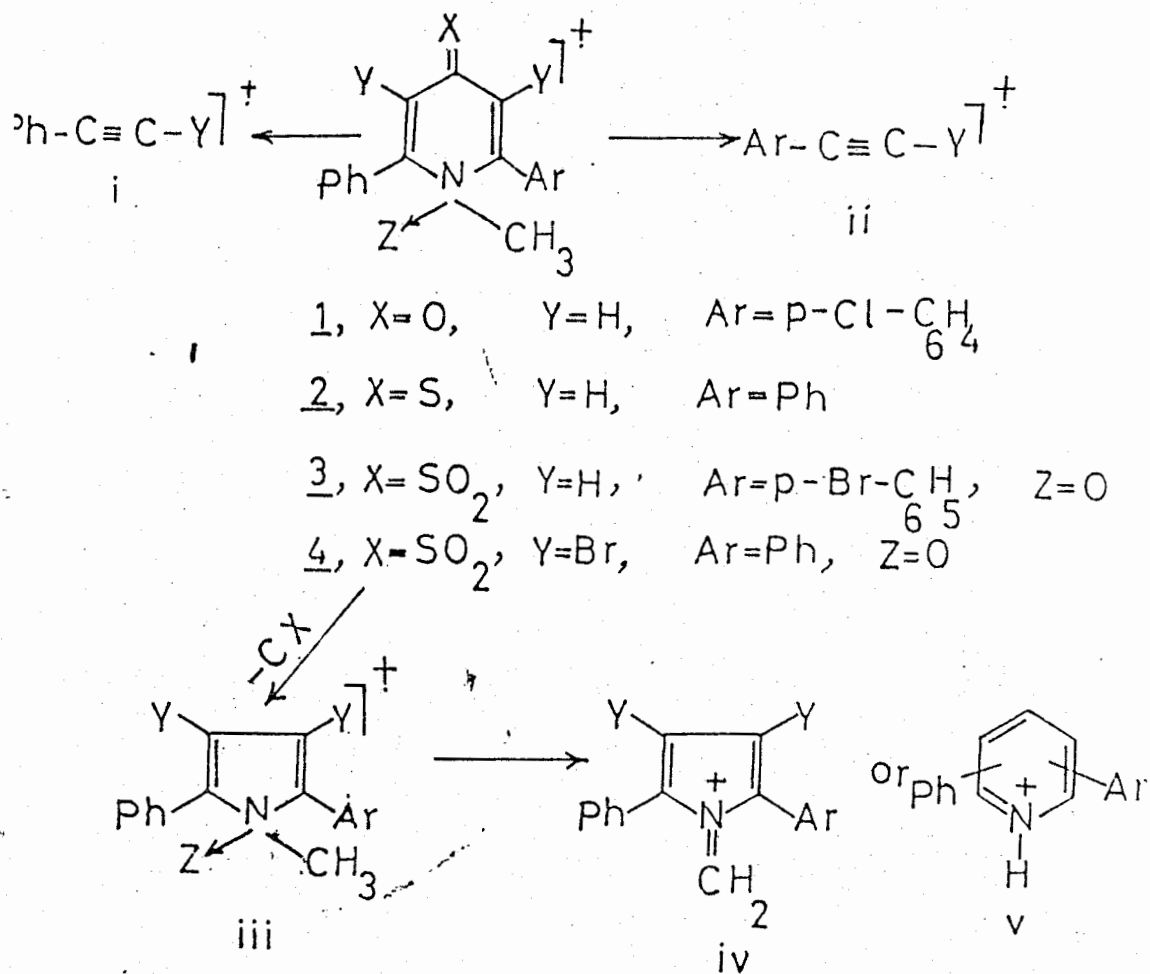
Anal . Calcd . for C₁₈H₁₃Br₂NO₃S : C, 44.7; H, 2.7 ; Br, 33.1 N,2.9; S, 6.6. Found : C, 44.9; H, 2.8; Br , 32. 7; N, 3.0;S, 6.8.

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Scheme

دراسة طيف الكتلة لبعض مركبات ٢، ٦ - ثنائى
أريل - ٤ - بيريدونات ومشتقاتها

الكبريتية المتشابهة

محمد جابر سرعى

قسم الكيمياء - كلية العلوم - جامعة الاسكندرية

الابراهيمية - الاسكندرية

لقد تبين من دراسة ومقارنة طيف الكتلة لبعض مشتقات البيريديونات التى تم
دراستها أهمية دورها فى اثبات التركيب الهيكلى وكذلك تميز طيفها الكتلنى عن
البيريديونات الاصل .