

ChemTech

International Journal of ChemTech Research

CODEN (USA): IJCRGG ISSN: 0974-4290 Vol.8, No.2, pp 869-877, **2015**

The mass spectral fragmentation of bis-aciridinediones and pyrazoloacridines derivatives

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Abstract: All the mono-acridinediones compounds (1-2) the electron ionization (EI) spectra are very clean, being dominated by loss of atoms or radicals such as CO,CH₃, ketene, isobutylene. The 9,9'-bisacridinedione fragmented into the mono-acridinediones followed by further general pattern characteristic of 9-substitued mono-tacridinediones. For the 10,10'acridinediones fragmentations occur so as to give acridinedione moieties, followed by the loss of CO as observed in the monoacridine system. In the case of pyazoloacridine derivatives, loss of H and HCN was observed from the compounds derived from dihydroresorcinol and loss of H, CH₃ due to presence of methyl groups was observed from the compounds derived from dimedone. In this paper, we would like to report the mass spectral fragmentation 10,10'-bisacridinediones (**3a-c**), 9,9'-bisacridinediones(**4a-b**) and mono and bis-pyrazoloacridine derivatives (**5 a-d,6 e-g,7**). **KeyWords**: Acridinedione, pyrazoloacridine, dihydroresorcinol, dimedone, ketene,

isobutylene, methyl group.

Introduction

Mass spectrometry (MS) is unequivocally a powerful tool of characterization of organic compounds. Several series of bis-acridinediones and pyrazoloacridines derivatives have been investigated by EI mass spectrometry because of due to their versatile wide applications such as laser dyes¹⁻⁸, OLED properties⁹, solar cell¹⁰ andbiological activities¹¹. The 9,9'-bisacridinedione(**4a-b**) fragmented into the mono-acridinediones followed by further general pattern characteristic of 9-substitued mono-tacridinediones. For the 10,10'acridinediones(**3a-c**), fragmentations occur so as to give acridinedione moieties, followed by the loss of CO as observed in the mono-acridinediones system. For mono, bis-pyrazoloacridines systems we have observed that the molecular ion was base peak for compounds **5a-d** derived from dihydroresocinol. Whereas, for dimedone derived compounds **6a-c**, 7, the base peak was the ion obtained from the molecular ion by loss of a methyl group from that gem-dimethyl groups. Loss of H and HCN was observed from compounds**5a-d** from the molecular ion. For the compounds **6a-c** and 7, these were a loss of H, CH₃ due to presence of methyl groups.

Experimental

The mass spectra were recorded with Jeol-JMS-DX 303 HF and GCMS QP 5000 Shimadzu instruments.

In this paper would like to report the mass spectral fragmentation 10,10'-bisacridinediones (3a-c), 9,9'bisacridinediones(4a-b) and mono and bis-pyrazoloacridine derivatives (5 a-d,6 e-g,7). The fragmentations of 10,10'-bisacridinediones3a, 3b, 3c were depicted(Table –I, Scheme –I). In general, the molecular ion was not detected (except 3a). The fragmentations occur so as to give acridinedione moieties, followed by the loss of CO as observed in the mono system. The 9,9'-bisacridinedione fragmented into the monoacridinediones followed by further general pattern characteristic of 9-substitued acridinediones.



10,10'- Bisacridinediones



3 a-c

Table - I

Compound	R	R [']	n
3a	CH ₃	Н	4
3b	CH ₃	C_3H_7	4
3c	Н	Н	4







The 9,9' - bisacridinedione fragmentations are explained as given below, for compounds 4a, 4b. Here again, the initial fragmentation occurs to result in two acridinedione units followed by the general pattern (Table – II, Scheme-II).

9,9' - Bisacridinediones





Table - II

Compound	R	
4a	Н	
4b	CH ₃	



Scheme - II



Mass spectra for mono and bis-pyrazoloacridines were studied (**Table III, IV**, **Scheme-III,IV**). It has been observed that the molecular ion was the base peak for compounds**5a-d** derived from dihydroresocinol. Whereas, for dimedone derived compounds **6a-c,7**, base peak was obtained from molecular ion by loss of a methyl group from that gem-dimethyl groups. Loss of H and HCN was observed from the compounds **5a-d** from the molecular ion. For the compounds **6a-c** and **7**, these were a loss of H, CH_3 due to presence of methyl groups. As commonly observed in acridinedione systems that the mass spectral fragmentations of **7** shows loss of isobutylene and ketene, due to presence gem-dimethyl groups and carbonyl group (**Scheme-VII**).



Table -	Ш
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Compound	R	Ŕ	R ″
5a	Н	Н	Н
5b	Н	Н	C_6H_5
5c	Н	CH ₃	Н
5d	Н	CH ₃	C ₆ H ₅



Table - IV

Compound	R	Ŕ	R″
6a	CH ₃	Н	Н
6b	CH ₃	Н	C ₆ H ₅
6c	CH ₃	CH ₃	Н





For compound **5c** $(m/z \ 277 \ M^+)$ the loss of H gives rise to $m/z \ 276$ peak, which on further fragmentation gives rise to $m/z \ 249$ signal (by the loss of HCN), which then leads to $m/z \ 205$ signal, similar to compound **5a**.

The methyl radical loss from the gem-dimethyl group but 12-methyl group fragmentation does not occur from compound **6c**.



Scheme- IV

Conclusion

Totally **13**bis-acridinediones andpyrozoloacridines derivatives were studied for their mass spectral fragmentations. Molecular mass information and fragmentation pattern are easily obtained under the electron ionization (EI) condition. Common fragment at m/z 272 (or 273) has also been recognized from most of theacridinediones, by loss of substituents at 9, 10 and gaining one H⁺. In the case of 10,10'-bisacridinediones, the molecular ion was not detected (except **3a**). The 9,9'- bisacridinedione fragmented into mono acridinediones followed by the further general pattern characteristic of 9-substitued acridinediones. In the case of dimedone derived compounds pyrazoloacridines**6a-c**,**7**, base peak was obtained from molecular ion by loss of a methyl group from that gem-dimethyl groups.

Acknowledgment

We thank the DST, India for the financial support of this work and Prof V.T. Ramakrishnan for generous support for all my work.

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