SCIENCE AND INNOVATION
INTERNATIONAL SCIENTIFIC JOURNAL VOLUME 3 ISSUE 2 FEBUARY 2024
UIF-2022: 8.2 | ISSN: 2181-3337 | SCIENTISTS.UZ

STUDY OF FRAGMENTATION OF BIS-CARBMATE MEE-2 INTO FRAGMENT IONS IN THE LIQUID CHROMATOGRAPHY-MASS SPECTRUM

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https://doi.org/10.5281/zenodo.10667029

Abstract. *In this research work, the mass spectra of N, N'-hexamethylene-bis-[(m-cresolyl)-carbamate], i.e. MEE-2, were studied. During the fragmentation of bis-carbamate, ions such as m-methylphenyl, hexamethylenediamine, carbamate and others appeared. As a result, ions were identified that proved the elemental composition, molecular weight, chemical bonds, brutto and structural formula of MEE-2 bis-carbamate.*

Keywords: *bis-carbamate, amine, hexamethylene, fragmentation, spectrum, bond, ions, molecule, atom, structure.*

Introduction. Molecules containing the carbamate group play an important role in the development of modern drugs, medicines and chemicals. Carbamate and bis-carbamate derivatives are widely used in agricultural chemicals such as pesticides, fungicides, acaricides and herbicides [1]. They also play an important role in the chemical and paint industries as starting materials, intermediates and solvents [2].

The authors of this article synthesized bis-carbamates of the MEE series. Also, physicochemical, biological and pharmacological parameters were studied and used in various branches of the chemical industry [3-5]. Below is the linear and three-dimensional structure of bis-carbamate MEE-2 (Figure 1):

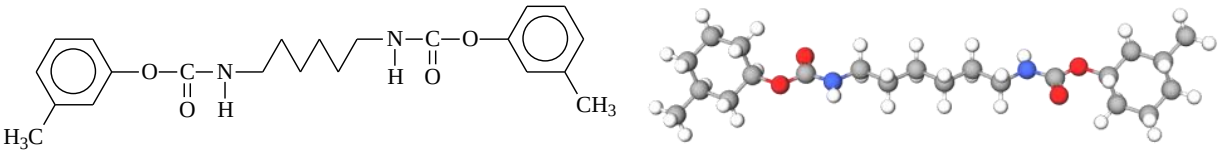


Figure 1. N,N'-hexamethylene-bis-[(m-cresolyl)-carbamate], i.e. MEE-2

The purpose of this research work is to study the structure of N,N'-hexamethylene-bis-[(m-cresolyl)-carbamate], i.e. MEE-2 with use mass spectroscopic method.

Materials and Methods. Chromato-mass spectrum of N,N′-hexamethylene bis-[(meta-cresolyl)-carbamate] i.e. MEE-2 on an Agilent Technologies 6420 spectrometer, APCI METHOD C118-brand column, 5% phenylmethylsilicone liquid phase, control parameters 500 °C initial temperatures ranging from 150 °C to 320 °C were obtained with an Agilent Technologies 9973 inert mass spectrometer.

Results and Discussions. In the chromato-mass spectrum of N,N′-hexamethylene bis-[(meta-cresolyl)-carbamate] i.e. MEE-2, the formation of ions corresponding to their molecular mass and the mass of fragment ions resulting from their fragmentation was determined (Fig. 2).

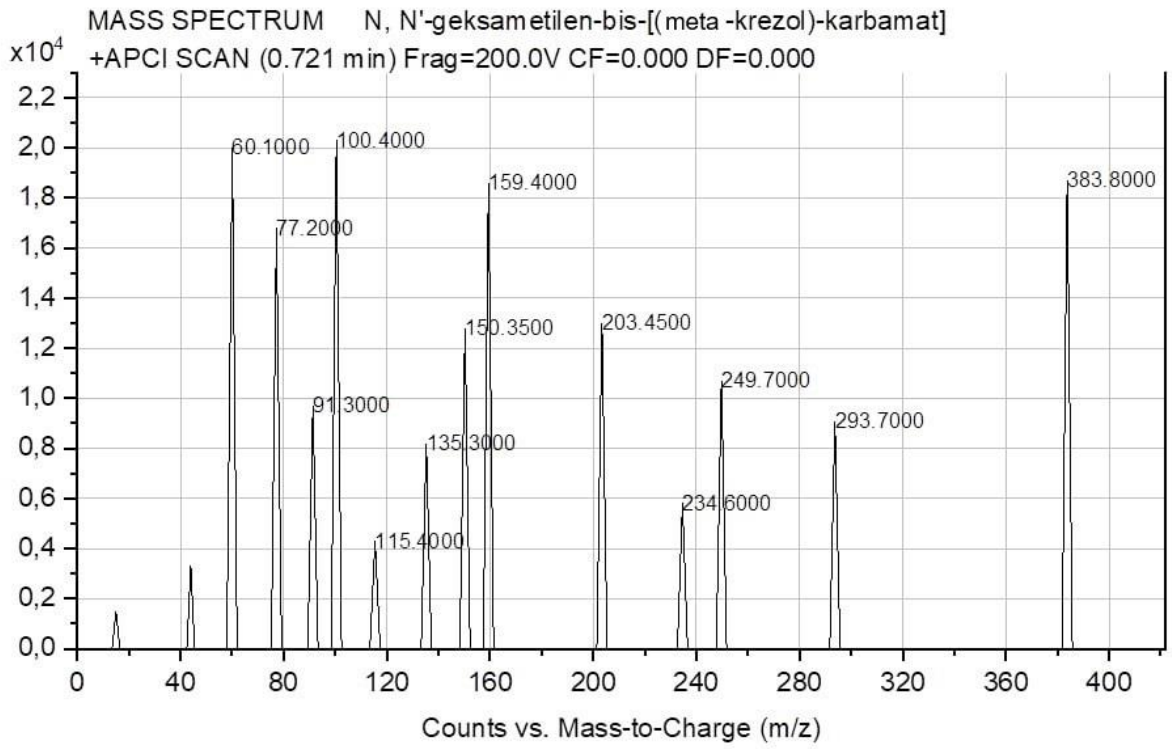
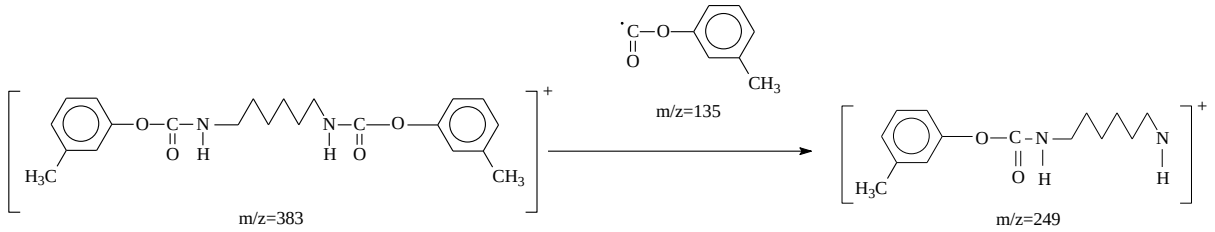


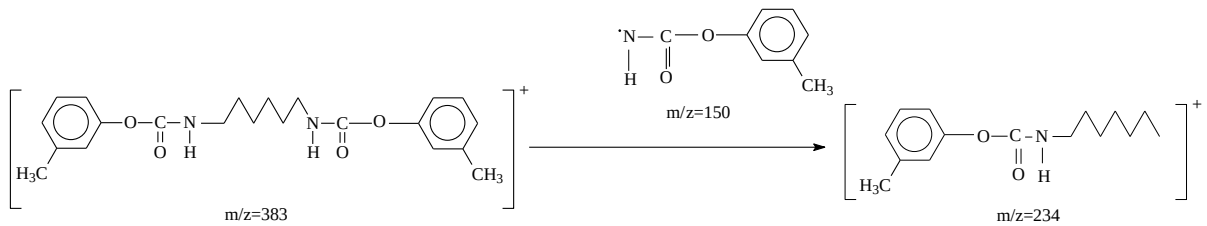
Figure 2. Chromato-mass spectrum of N,N'-hexamethylene bis-[(meta-cresolyl)-carbamate] i.e. MEE-2

In this case, the molecular ion peak of MEE-2 was equal to 383.8. Above is the chromato-mass spectrum of fragment ions formed from the initial MEE-2 molecular ion (Fig. 2). In addition, in the spectrum, mass m/z 249, m/z 135, m/z 91, in the second direction, m/z 234, m/z 100, in the third direction, m/z 293, m/z 249, formation of fragment ions with m/z 202, m/z 158, m/z 114 and m/z 59 was determined.

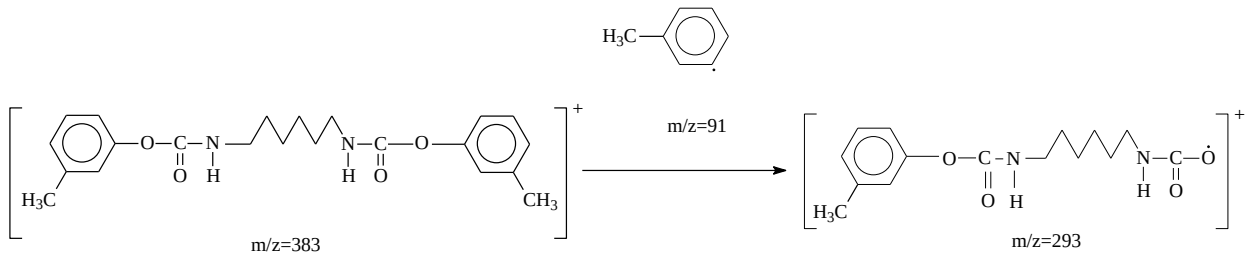
After the MEE-2 substance was included in the chromato-mass spectrum, a bis-carbamate molecular ion with m/z 383 was formed in 0.711 minutes under the selected conditions. In turn, the MEE-2 ion with m/z 249 from the release of the m/z 135 radical in one direction at 0.183 minutes from the bis-carbamate ion:



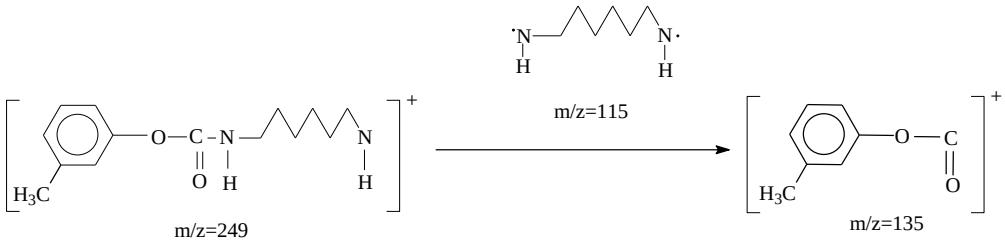
In the second direction, the MEE-2 ion with m/z 234 splits off at 0.192 minutes with m/z 150 radical:



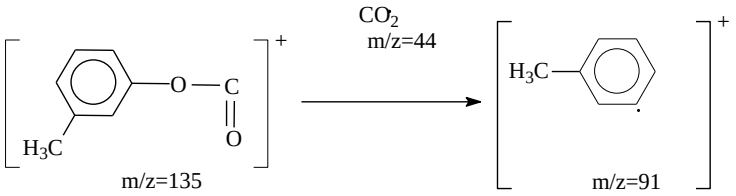
In the third direction, the separation of MEE-2 ions with m/z 293 from the release of the m-methylphenyl radical at 0.185 minutes was shown:



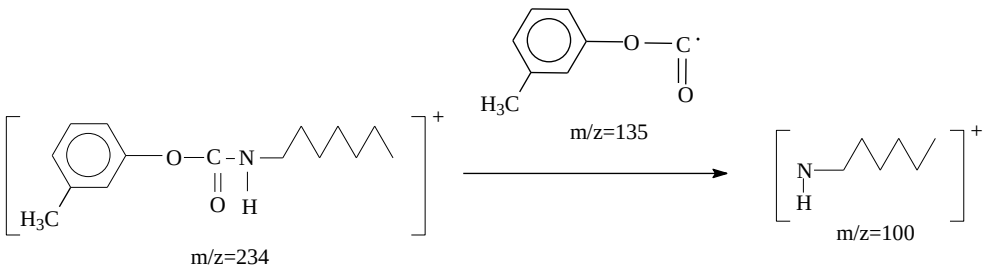
In the chromato-mass spectrum, fragment ions formed from molecular ions also form small ion fragments. The m/z 249 ion formed from MEE-2 separated from itself the hexamethylenediamine radical with m/z 115 to form the ion with m/z 135:



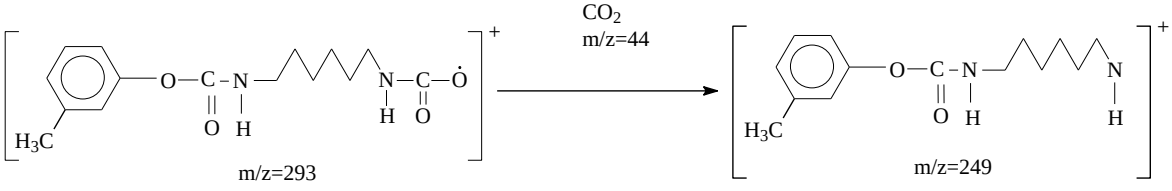
The resulting m/z 135 ion separated from itself a carbon dioxide molecule with m/z 44 and formed an ion with m/z 91:



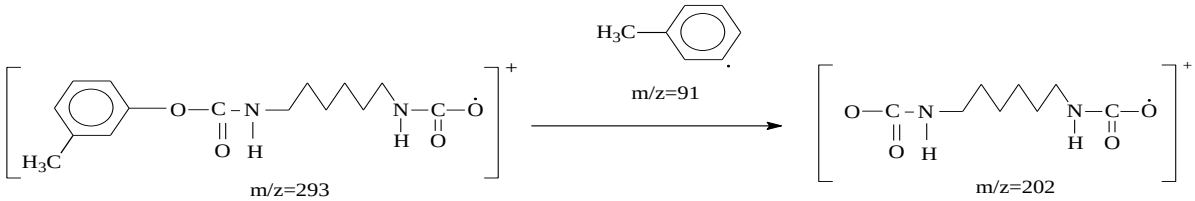
The ion formed in the second direction of the initial MEE-2 ion separates the m/z 135 radical from it and forms an ion with m/z 100:



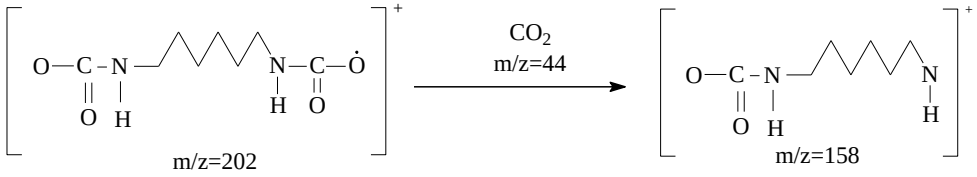
The m/z 293 ion formed in the third direction of the molecular ion of MEE-2, in its turn, disintegrates in two directions. In the first direction, m/z 44 separates carbon dioxide and forms an ion with m/z 249:



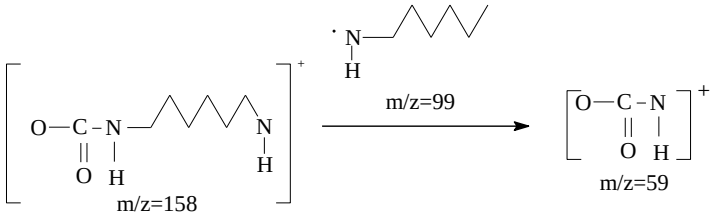
The second m-methylphenyl radical with m/z 91 is separated from the m/z 249 ion, forming the N,N-hexamethylene bis-carbamate ion with m/z 202:



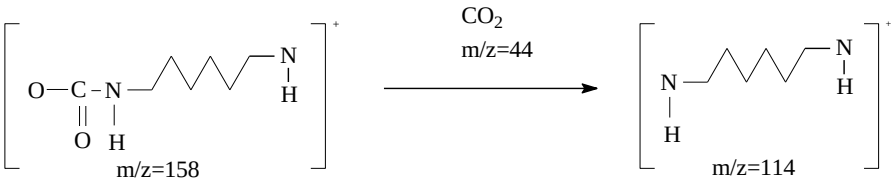
The resulting m/z 202 N,N-hexamethylene bis-carbamate ion separates from itself a m/z 44 carbon dioxide molecule and forms an ion with m/z 158:



The m/z 158 ion also fragmented in two directions. In the first direction, he separated the hexamethyleneamine radical with m/z 99 from itself and formed the carbamate ion with m/z 59:



In the second direction, it separated carbon dioxide m/z 44 from itself and formed N,N-hexamethylenediamine ion with m/z 114:



The above listed fragments of the MEE-2 molecule prove the composition, structure and brutto formula of the synthesized bis-carbamate.

Conclusion. Upon fragmentation of the N,N'-hexamethylene-bis-[(m-cresolyl)-carbamate] molecule, i.e. MEE-2 chromatography-mass spectroscopy method identified ions such as m-methylphenyl, hexamethylenediamine, carbon dioxide, N,N-hexamethylene bis-carbamate, carbamate itself and others. These fragments prove the structure of bis-carbamate MEE-2.

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