International Journal of Mass Spectrometry 273 (2008) 20–23

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

Electron impact ionization of acetaldehyde

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ARTICLE INFO

Article history:
Received 11 February 2008
Accepted 13 February 2008
Available online 10 March 2008

PACS:
34.80.Gs

Keywords:
Acetaldehyde
Electron impact
Ionization energy
Appearance energy

ABSTRACT

An electron impact (EI) ion source and a double focusing sector field mass spectrometer were used to investigate ionization processes of acetaldehyde C_2H_4O. The ionization and appearance energies for observed single $C_xH_yO_z^+$ ($x = 0, 1, 2$; $y = 0, 1, \ldots, 4$; $z = 0, 1$) and double $C_2H_2O^{2+}$ charged ions have been determined by using the non-linear least-square fitting procedure to the raising set of the data points. In the case of ions C_2HO^+, C_2O^+, CH_3O^+, CH_2O^+, $C_2H_2^+$, C_2H^+, C_2^+, H_2O^+, HO^+ and $C_2H_2O^{2+}$ the appearance energies were obtained for the first time.

1. Introduction

Acetaldehyde C_2H_4O is very important molecule from the scientific and applied points of view. It occurs naturally in ripe fruit, coffee and fresh bread and is produced by plants as a part of their natural metabolism. This molecule is an air pollutant resulting from combustion, such as automotive exhaust fumes and tobacco smoke, contributing to the addictive properties of tobacco [1,2]. Investigation of ionization processes of acetaldehyde is being a subject of studies of many investigators within last few decades. For these investigations, and especially for determination of appearance energies of acetaldehyde fragment ions several measurement techniques were applied (EI, electron impact; PI, photoionization; PE, photoelectron spectroscopy; S, optical spectroscopy; PIPECO, photoion–photoelectron coincidence spectroscopy). Most of them concern the ionization energy of pattern ion $C_2H_4O^+$. For the wide spectrum of observed fragment ions created during the fragmentation in the ion source not every values of appearance potentials are reported.

In our laboratory observations of metastable fragmentation reactions of ions produced by electron impact of molecules play a special role [3–9]. Just absence of metastable fragmentation reactions of acetaldehyde ions was for us direct encouragement for the investigations presented here.

Therefore, in this work mass spectrometric investigations of ionization or appearance energies for all observed acetaldehyde ions produced by electron impact are presented. To our knowledge, this is the first time that threshold and appearance energies for all observed ions from electron impact of acetaldehyde have been measured on the apparatus using the same method.

2. Experimental

A high-resolution double focusing sector field mass spectrometer of reversed Nier–Johnson-type B–E geometry with the Nier-type electron impact ion source was applied for investigations presented here (Fig. 1). This spectrometer is an improved version of the MX 1321-type spectrometer used by us for investigations of ionization processes in gasses and gaseous clusters and was described in detail previously [10–12]. This apparatus is equipped with a channeltron-

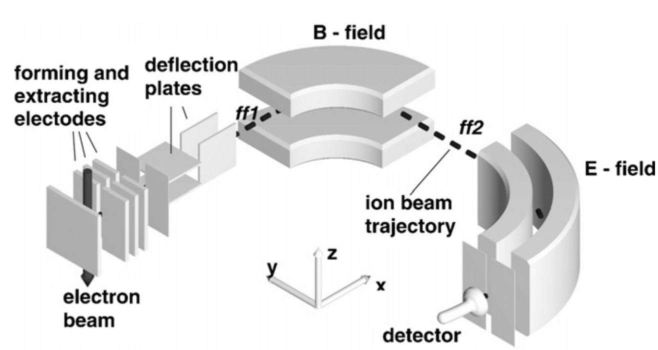

Fig. 1. Schematic view of the double focusing sector field mass spectrometer of reversed Nier–Johnson-type B–E geometry.

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doi:10.1016/j.ijms.2008.02.006

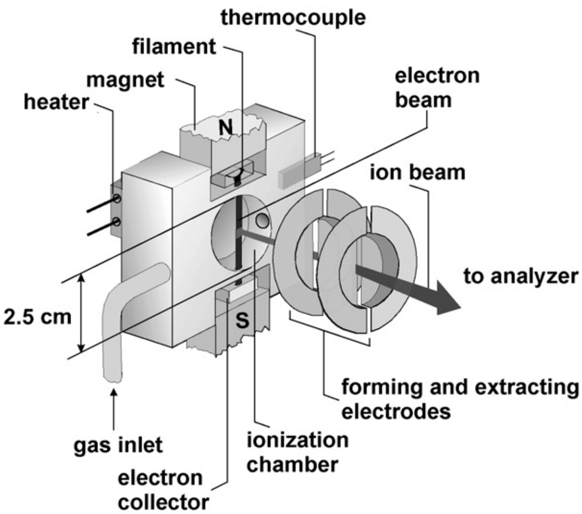

Fig. 2. The electron impact ion source.

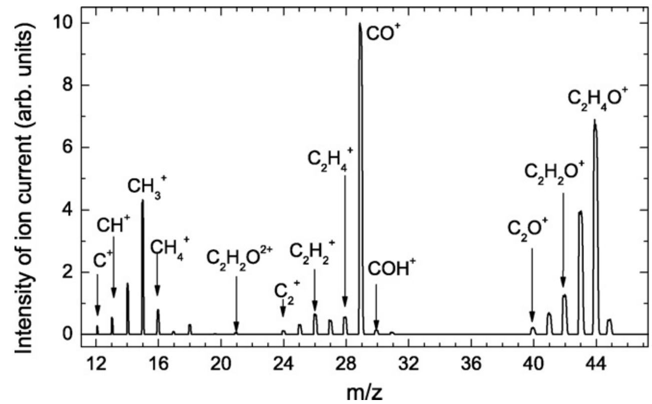

Fig. 3. Electron impact mass spectrum of acetaldehyde. The electron ionization energy E_e = 100 eV and the intensity of electron beam I_e = 0.3 mA.

type-based detection system and the vacuum system allows to work with a background pressure of 4×10^{-8} mbar.

The schematic view of electron impact ion source is presented in Fig. 2. In the ionization chamber a magnetic field (magnet) is parallel to the electron beam axis. The electron energy is scanned in an automated stepwise mode with the energy increment of 0.1 eV starting from 0 up to 100 eV. In the present experiment the electron beam current was set up to 0.3 mA. The maximum electron current can be set up to 1.0 mA. The ion source pressure is controlled by a Balzers Compact Full Range

Table 1
Ionization and appearance energies

Ion	Other products	Ionization or appearance energies (eV)		
		This work	Method	Literature
$C_2H_4O^+$		10.20 ± 0.1	EI	10.23 [33]; 10.14 ± 0.02 [34]
			PI	10.20 ± 0.03 [19]; 10.21 ± 0.01 [20]; 10.25 ± 0.03 [21]; 10.20 ± 0.03 [22]; 10.22 ± 0.01 [23]; 10.20 ± 0.02 [24]; 10.22 ± 0.01 [25]; 10.20 ± 0.02 [26]; 10.22 ± 0.01 [27]; 10.2298 ± 0.0007 [28]; 10.20 [29]; 10.22 [30]; 10.22 [31]; 10.22 [32]
			PE	10.20 [35]; 10.22 ± 0.01 [36]; 10.24 ± 0.02 [37]; 10.21 [38]; 10.26 [39]; 10.20 [40]; 10.9 [41]; 10.20 [42]; 10.227 ± 0.005 [43]; 10.23 [44]; 10.3 [45]
			S	10.2291 ± 0.0007 [17]; 10.19 [18]
			PIPECO	10.24 [46]
$C_2H_3O^+$	H	11.00 ± 0.1	EI	10.5 ± 0.2 [47]; 10.75 ± 0.08 [48]; 11.0 ± 0.1 [50]; 10.67 [31];
			PI	10.89 [23]; 10.89 ± 0.03 [25]; 10.90 ± 0.03 [27]; 10.82 ± 0.03 [26]; 10.82 [29]; 10.90 [30]
			PIPECO	10.50 ± 0.05 [49]
$C_2H_2O^+$	H_2	12.70 ± 0.1	EI	10.7 ± 0.1 [23]
			PI	13.06 ± 0.09 [27]
C_2HO^+	H_3	14.20 ± 0.1	EI	
C_2O^+	H_2H_2	13.50 ± 0.2	EI	
CH_3O^+	CH	13.50 ± 0.2	EI	
CH_2O^+	CH_2	11.80 ± 0.2	EI	
CHO^+	CH_3	12.20 ± 0.1	EI	
			PI	11.78 [32]; 11.79 ± 0.03 [26]; 11.79 ± 0.03 [24]
$CO^+/C_2H_4^+$	CH_4/O	11.90 ± 0.15	EI	13.9 ± 0.1 [47]; 14.0 ± 0.1 [47];
$C_2H_3^+$	OH	15.60 ± 0.2	EI	14.17 ± 0.13 [27];
$C_2H_2^+$	HOH	15.40 ± 0.2	EI	
C_2H^+	H_2+OH	22.70 ± 0.2	EI	
C_2^+	H_2+HOH	32.00 ± 0.2	EI	
$C_2H_2O^{2+}$	H_2	29.30 ± 0.4	EI	
HOH^+	C_2H_2	10.90 ± 0.2	EI	
HO^+	C_2H_3	10.60 ± 0.2	EI	
CH_4^+/O^+	CO/C_2H_4	12.80 ± 0.1	EI	
			PI	12.61 ± 0.06 [27]; 12.61 [30]
CH_3^+	CHO	13.30 ± 0.1	EI	14.53 [51];
			PI	14.11 ± 0.05 [26]; 14.08 ± 0.05 [27]; 14.08 [30]
			PIPECO	13.9 ± 0.1 [49]
CH_2^+	CH_2O	18.50 ± 0.1	EI	
			PI	15.08 ± 0.09 [27]
CH^+	C_2H_3O	20.60 ± 0.1	EI	
C^+	CH_4O	21.40 ± 0.2	EI	

EI, electron impact; PI, photoionization; PE, photoelectron spectroscopy; S, optical spectroscopy; PIPECO, photoion–photoelectron coincidence spectroscopy.