Investigation of Molecular Ions of Some Benzyl Derivatives Using Deconvolution Technique

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ABSTRACT. The ionization energies at threshold and values of higher energy levels for the molecular ions of benzyl alcohol, benzyl amine and benzyl cyanide are reported using electron impact technique. The first ionization energy values are found to be 8.26 eV (benzyl alcohol), 8.49 eV (benzyl amine) and 9.32 eV (benzyl cyanide). Some of the reported higher energy levels for the molecular ions are tentatively explained. The differences in the relative abundances for the main fragment ions are also discussed and attributed to the effect of $-OH$, $-NH_2$ and $-CN$ groups.

Ionization and fragmentation of benzyl compounds have been of interest to mass spectrometrists. The ionization energy for benzyl alcohol, benzyl amine and benzyl cyanide had been measured at threshold only (Pignataro *et al.* 1966, Russeell *et al.* 1983, Dekock *et al.* 1983, Watanabe and Mottl 1957, Vilesov and Terenin 1957, Akopyan and Vilesov 1964, Van der Greef 1979). On the other hand, the probable mechanisms for formation of the main fragment ions from the three mentioned molecules are dependent upon the substituent groups. Therefore, it is necessary to make correlation between mass spectra and energy considerations.

In the present study we have examined the molecular ions (for 4 eV above threshold) of benzyl alcohol, benzyl amine and benzyl cyanide. The electron impact technique is used for measuring the ionization efficiency (IE) curves for the ions studied. By using the deconvoluted first differential (DED) technique (Selim 1985) we have been able to study the ionization energies at threshold, as well as

studying higher energy states for the three studied molecular ions. The DFD technique have proved (Selim and Helal 1982, Selim et al. 1984, Selim et al. 1987, Selim et al. 1987) to be useful for studying IE curves obtained by electron impact and the results obtained are sufficiently accurate for comparison with similar results.

Also, the effect of different groups ($-OH$, $-NH_2$ and $-CN$) on the ionization energies of the title molecules, as well as on the relative abundance of main fragment ions produced from the molecules have been discussed.

Experimental Technique

Ionization efficiency data are obtained using an Atlas CH-4 mass spectrometer with a normal electron impact (AN-4) ion source. The conditions of measurements and the method of calibration of the electron energy scale are the same as reported previously (Selim 1976). The draw-out potential is always set at zero value in order to increase the residence time in the ion source, which favours the detection of low energy processes. The electron energy is varied in 0.1 eV steps using a 10 turn helipot potentiometer and is measured with a digital multimeter Model DM2 of the Sinclair Radionics Limited.

The directly measured IE curves are smoothed by a 5-point smoothing (Savitzky and Golay 1964) computer technique in order to decrease the random noise in the raw data. Once again using a computer technique the smoothed data are treated (Savitzky and Golay 1964) to obtain the first derivative IE curves, and then the inverse convolution technique of Vogt and Pascual (Vogt and Pascual 1972) is applied to obtain the deconvoluted IE curves. Details of the application of this combined technique have been reported elsewhere (Selim et al. 1985).

Results and Discussion

The DFD IE curves (corrected) for the molecular ions, studied up to 44 eV above threshold, are given in Figs. 1-3. The ionization energies and higher energy electronic states (levels) obtained from the three molecular ions, together with similar results (at threshold only) reported previously by other authors using different techniques, are reported in Table (1). The values given in Table (1) are the average of 8 determinations and the errors quoted are the standard deviations. Only reproducible values are reported in the table.

The relative abundances (relative to base peak) of the molecular ions and the main fragment ions from the three molecules are listed at 70 and 14 eV in Table

(2). The fragmentation pathways are nearly similar as shown in chart 1, however, the quantitative differences are appearan from Table (2).

Molecular Ions

The three molecular ions under consideration are all monosubstituted toluenes having the formula $[C_6H_5CH_2X]^+$, where X = OH, NH_2 and CN respectively. However, during the present discussion for the molecular ions, the presently studied molecules are treated as monosubstituted benzenes with substituent groups: CH_2OH, CH_2NH_2 and CH_2CN respectively.

Benzyl Alcohol Molecular Ion $[C_7H_8O]^+(m/Z = 108)$

The DFD IE curve shows a sharp rise at threshold which may indicate that the adiabatic ionization energy coincides with the vertical ionization energy. The ionization energy of benzyl alcohol at threshold is measured at 8.26 ± 0.05 eV and is in good agreement with electron impact value (8.34 eV) reported recently by Russell *et al.* (1983). An electron impact value (9.14 eV) reported early by Pignataro *et al.* (1966) probably does not correspond to the first ionization energy. In fact, the latter value corresponds to an energy level measured by us at 9.09 eV.

Table 1. Ionization energies and higher energy levels (eV) for benzyl alcohol, benzyl amine and benzyl cyanide molecular ions

Benzyl alcohol [C₇H₈O]′		Benzyl amine [C₇H₉N]′		Benzyl cyanide [C₈H₇N]′	
This work	Literature	This work	Literature	This work	Literature
			7.56 ± 0.02[a]		
8.26 ± 0.05	8.34[b], 8.90[c]	8.49 ± 0.06	8.64 ± 0.02[c]	9.32 ± 0.05	9.34[d]
9.09 ± 0.06	9.14 ± 0.05[f]	9.12 ± 0.13	9.03 ± 0.05[c]	10.15 ± 0.14	9.40 ± 0.05[e]
9.66 ± 0.12	9.53[g]	9.46 ± 0.10	9.46[f]	10.71 ± 0.08	
10.03 ± 0.12	10.3[c]	9.97 ± 0.14		11.02 ± 0.09	
10.62 ± 0.13	−	10.44 ± 0.09		11.34 ± 0.08	
11.13 ± 0.15	11.20[c]	10.98 ± 0.08		11.88 ± 0.12	
11.76 ± 0.12	11.70[c]	11.40 ± 0.08		12.44 ± 0.14	
12.14 ± 0.15	12.40[c]	11.80 ± 0.13		13.14 ± 0.13	
		12.49 ± 0.12			

(a) Watanabe and Mottl (1957),
(b) Russell *et al.* (1983),
(c) Akopyan and Vilesov (1964),
(d) Van der Greef *et al.* (1979),
(e) Pignataro *et al.* (1966), and
(f) DeKock *et al.* (1983).

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A photoelectron value at 9.53 eV reported recently by Dekock *et al.* (1983) had been assigned by them to ionization of electron from $A_2\pi$ orbital of the benzene ring. An energy level has been measured by us at 9.66 eV is corresponding within experimental errors-to the ionization energy value reported by Dekock *et al.* (1983).

Table 2. Relative intensities of the main ions from the three molecular ions at 70 and 14 eV

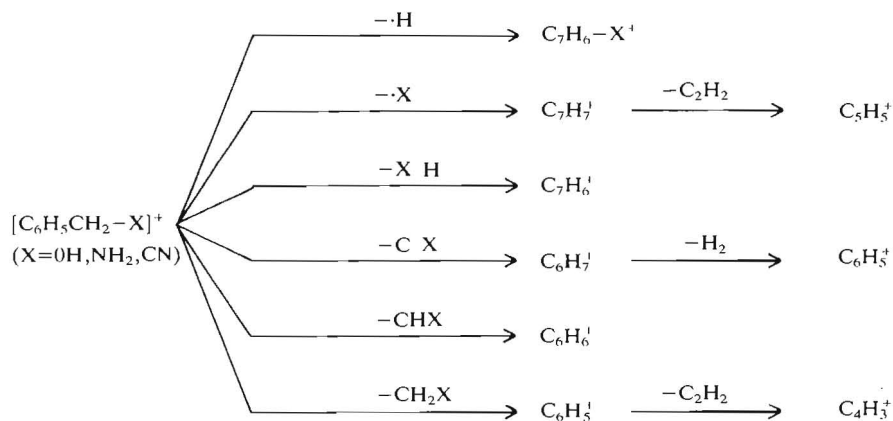| Ion Formula	Benzyl alcohol		Benzyl amine		Benzyl cyanide	
	70eV	14eV	70eV	14eV	70eV	14eV
M^+	93.2	100	68.4	80.6	100	100
$M-1^+$	83.7	66.3	100	100	32.1	1.8
$C_7H_7^+$	39.7	11.8	19.4	8.3	8.6	0.5
$C_7H_6^+$	20.5	6.6	3.3	1.1	38.9	3.8
$C_6H_7^+$	100	75.4	45.4	13.4	1.9	—
$C_6H_6^+$	29.2	5.7	17.7	5.6	1.8	—
$C_6H_5^+$	80.3	17.0	24.3	2.8	8.3	0.4
$C_5H_5^+$	17.2	—	8.3	—	4.8	—
$C_4H_3^+$	52.0	—	22.9	—	14.8	—

Chart (1) The main fragmentation processes for the three molecular ions.

The value[*] 8.26 eV, for the ionization energy of benzyl alcohol at threshold, is lower by about 1 eV than the first ionization energy of benzene (El-Sayed *et al.* 1961). This lowering in ionization energy is probably due to the substitution effect of CH_2OH group. If the degeneracy of $^2E_{1g}$ ground state of benzene positive ion is removed (Turner *et al.* 1970) by the substitution of CH_2OH group (as might be expected) then, one may assume that the ionization energy 8.26 eV is due to ionization of $1e_{1g}$ electron from π_3 (B_1 component) orbital. Consequently, the level
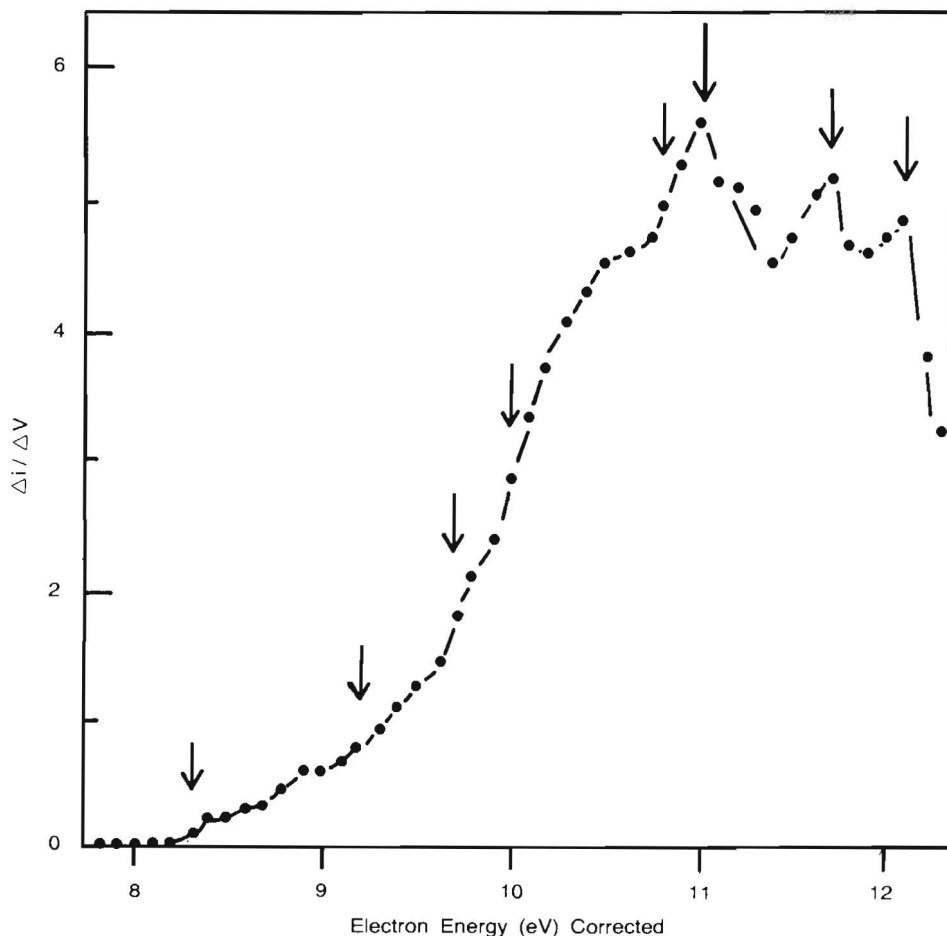

Fig. 1. The deconvoluted first differential IE curve for benzyl alcohol molecular ion (m/z = 108).

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[*] Comparing the ionization energy at threshold for benzyl alcohol with that of toluene (Selim and Helal 1982) indicates that replacement of the methyl group hydrogen by OH leads to the ionization energy of toluene being decreased by 0.54 eV.

at 9.09 eV is tentatively considered as due to ionization of le_{1g} electron from π_2 (A_2 component) orbital. The two lowest ionization energies of benzyl alcohol molecular ion differ in energy by 0.83 eV in comparison with differences (Baker *et al.* 1968) 0.70 eV for phenol and 0.83 eV for anisol.

It has been concluded (Baker *et al.* 1968) that the ionization energy of $a_{2u}\pi_1$ electrons in benzene is 11.48 eV and the differences between π_1 orbital energy in benzene and substituted benzenes are often quite unlike the differences between π_3 orbitals. If one assumes that the ionization energy of the $a_{2u}\pi_1$ electrons in benezene molecular ion is lowered in benzyl alcohol molecular ion-due to the
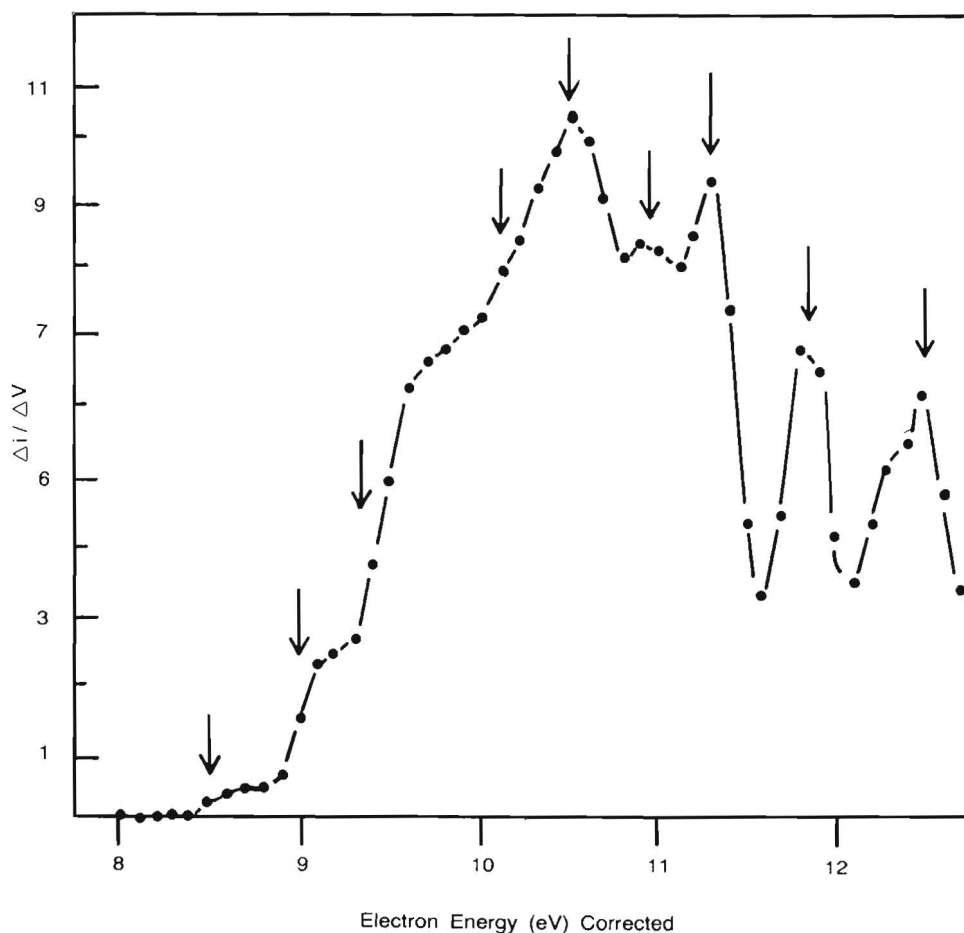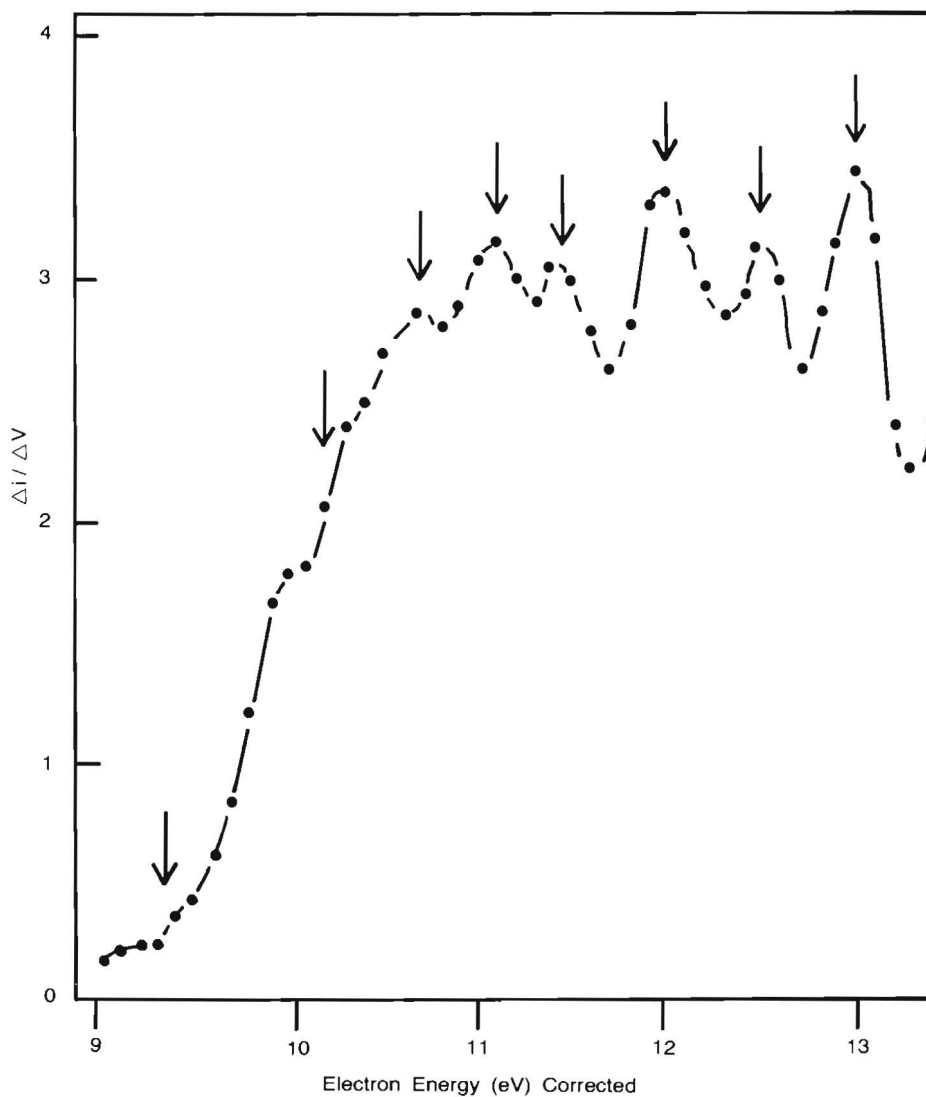

Fig. 2. The deconvoluted first differential IE curve for benzyl amine molecular ion (m/z = 107).

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due to the lone pair. As a result, one cannot discard the possibility that the level at 11.13 eV is due to ionization of 2p lone pair electrons of the oxygen atom, in CH_2OH substituent.

However, Ballard *et al.* (1986) had detected a peak (B band) at 10.3 eV in the photoelectron spectrum of the gas phase benzyl alcohol and assigned it to the vertical ionization energy of the non-bonding oxygen orbital. In fact, an energy level has been detected in the present work at 10.03 eV which may correspond to that peak reported by Ballard *et al.* (1986). Also, they found a peak at 11.20 eV which may correspond to the level reported by us at 11.13 eV. One may assume that the level at 10.03 eV is due to ionization of lone pair electron of oxygen and the level at 11.13 eV is due to ionization of a_{2u} electron from π_1 orbital.

Three energy levels measured, by the present authors, at 9.66, 10.62 and 11.76 eV are correlated within experimental errors - with the appearance energies (AE's) of $[C_6H_4O]^+$ ion at 9.51 ± 0.05 eV (Selim *et al.* 1989), $[C_7H_7O]^+$ ion at 10.46 ± 0.06 eV (Selim *et al.* 1987) and $[C_7H_7]^+$ ion at 11.76 ± 0.07 eV (Selim *et al.* 1987) (and probably also $[C_7H_7]^+$ ion at 11.71 ± 0.06 eV) (Selim *et al.* 1987). The levels at 9.66, 10.62 and 11.76 eV are probably predissociated and responsible for the formation of the corresponding fragment ions.

Finally a higher energy level has been measured in the benzyl alcohol IE curve at 12.14 eV. This level has an equivalent one (vertical) obtained by photoelectron spectroscopy (Ballard *et al.* 1986) at 12.40 eV. However, the level 12.14 eV cannot be explained in the present study.

Benzyl Amine Molecular Ion $[C_7H_9N]^+$ (m/Z = 107)

The presently reported DFD IE curve shows similarity, regarding the sharp rising at threshold, with the photoionization curve reported early by Akopyan *et al.* 1961). This sharp rise in the presently reported curve may indicate that the adiabatic ionization energy coincides with the vertical ionization energy. The ionization energy at threshold is 8.49 ± 0.06 eV which is in a good agreement with the photoionization value (8.64 eV) reported early by Akopyan and Vilesov (1964) but higher by about 1 eV than the earlier photoionization value reported by Watanabe and Mottl (1957). An electron impact value measured by Pignataro *et al.* (1966) at 9.03 eV probably does not correspond to the first ionization energy for the ion. The latter value corresponding - within experimental erros to the presently measured higher energy level at 9.12 eV. A photoelectron value at 9.46 eV reported recently by DeKock *et al.* (1983) had been assigned by them to ionization of electron from $A_2\pi$ orbital of the benzene ring. An energy level, measured by us, at 9.46 eV, corresponds exactly to the ionization energy value reported by the latter authors (DeKock *et al.* 1983).

The value* 8.49 eV, for the ionization energy of benzyl amine at threshold, is lower by about 0.76 eV than the first ionization energy of benzene (El-Sayed *et al.* 1961) (1 e_{1g} electrons). This lowering in ionization energy is probably due to the substitution effect of CH_2NH_2 group. Assuming the degeneracy of $^2E_{1g}$ ground state of benzene positive ion (Turner *et al.* 1970) is removed by substitution, one may suggest that the ionization energy 8.49 eV is due to ionization of 1 e_{1g} electron from π_3 (B_1 component) orbital. Consequently, the level at 9.46 eV is tentatively considered, similar to Dekock *et al.* (1983), as due to ionization of 1 e_{1g} electron from π_2 (A_2 component) orbital. The two lowest ionization energies of benzyl amine molecular ion differ in energy by 0.97 eV in comparison with difference 1.07 eV for aniline (Baker *et al.* 1968).

Assuming that the ionization energy of a_{2u} π_1 electrons in benzene molecular ion is lowered in benzyl amine molecular ion-due to CH_2NH_2 substitution in benzene one may attribute the level measured by us at 10.98 eV to ionization from π_1 a_{2u} orbital. It is worthwhile to mention that Akopyan *et al.* (1961) suggested early that ionization energy of π_1 orbital of benzyl amine apparently occurs at 2.2-2.4 eV above the threshold.

Three energy levels have been measured at 9.12, 11.80 and 12.49 eV. These levels correspond within experimental errors to AE's for $[C_7H_8N]^+$ (9.25 $\pm$ 0.06 eV), (Selim *et al.* 1987), $[C_7H_7]^+$ (11.75 $\pm$ 0.06 eV) (Selim *et al.* 1987) and $[C_7H_8]^+$ (12.47 $\pm$ 0.08 eV) (Selim *et al.* 1990) fragment ions respectively, obtained from benzyl amine. The levels 9.12, 11.80 and 12.49 eV are probably predissociated and may be responsible for the formation of $[C_7H_8N]^+$, $[C_7H_7]^+$ and $[C_7H_8]^+$ fragment ions, respectively.

Three more energy levels have been detected at 0.97, 10.44 and 11.40 eV. These levels cannot be explained in the present study.

Benzyl Cyanide Molecular Ion $[C_8H_7N]^+$ (m/Z = 117)

The DFD IE curve for the ion exhibits a sharp rise at threshold. The ionization energy at threshold is obtained at 9.32 $\pm$ 0.05 eV and is in good agreement with previously reported electron impact values at 9.34 eV (Van der Greef *et al.* 1979) and 9.40 eV (Pignataro *et al.* 1966).Our value**at 9.32 eV is higher by only 0.07 eV than the first ionization energy of benzene (El-Sayed *et al.*

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* Comparing the ionization energy at threshold for benzyl amine with that of toluene (Selim and Helal 1982) indicates that replacement of the methyl group hydrogen (of toluene) by NH_2 leads to the ionization energy of toluene being decreased by 0.31 eV.

** Comparing the ionization energy at threshold for benzyl cyanide with that of toluene (Selim and Helal 1982) indicates that replacement of the methyl group hydrogen (of toluene) by CN leads to the ionization energy of toluene being decreased by 0.52 eV.

1961). The closeness of the two values for the ionization energy may indicate that the substituent group CH_2CN has a negligible effect on the first ionization energy of benzene. However, it is well known (Turner *et al.* 1970) that monosubstituted benzenes, with electron-withdrawing substituents (like CN) attached directly with the benzene ring increase substantially the ionization energies of the monosubstituted benzenes relative to that of benzene. The ionization energy at threshold 9.32 eV is explained as due to ionization of one of the highest π electrons (e_{1g} electrons) of benzyl cyanide.

The photoelectron spectra (Turner *et al.* 1970) of monosubstituted benzenes, with electron-withdrawing substituents like C_6H_5CN and $C_6H_5CF_3$, show little or no loss of degeneracy of π_3 and π_2 orbital energy levels. Consequently, one may assume that in the case of benzyl cyanide molecular ion, no loss of the two fold degeneracy of $^2F_{1g}$ ground state of benzene ion is occurring, due to the presence of CH_2CN substituent.

A level has been measured at 11.34 eV and is tentatively assigned to ionization of a_{2u} electron from π_1 orbital of the benzene ring. Six more energy levels have been measured at 10.15, 10.71, 11.02, 11.88, 12.44 and 13.14 eV. One of these levels at 12.44 eV is correlated - within experimental errors - with AE of $[C_8H_6N]^+$ fragment ion at 12.46 ± 0.06 eV (Selim *et al.* 1987) obtained from benzyl cyanide.

The effect of different groups (OH, NH_2, CN) on stability of the molecular ions is illustrated by the relatively higher ionization energy at threshold of benzyl cyanide as well as its more intense peak (at 70 and 14 eV) relativel to the molecular ions of benzyl alcohol and benzyl amine. The order of decreasing stability of the molecular ions is benzyl cyanide > benzyl alcohol > benzyl amine. The greater stability of benzyl cyanide molecular ion (with electron - withdrawing group CN) may indicate the relatively lower internal energy of the ion and hence its lower fragmentation rate (lower rate constant) (Kiser 1965) relative to benzyl alcohol and benzyl amine (with electron - donating groups OH and NH_2). On the other hand, the difference in fragmentation processes is clear in loss of CHO from molecular ion of benzyl alcohol to form $[C_6H_7]^+$ ion, which represents the base peak at 70 eV, while the same ion $[C_6H_7]^+$ is formed at 70 eV with very low intensity (1.9%) in case of benzyl cyanide. Furthermore, the $[C_7H_6]^+$ fragment ion is formed by loss of HCN from molecular ion of benzyl cyanide with relative intensity 38.9% at 70 eV while, the same ion is formed from benzyl amine with very low intensity (3.3%). These differences are due to the effect of different groups (OH, NH_2, CN) on energy values, fragmentation processes and relative intensities of ions.

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دراسة الأيون الجزيئي لبعض مشتقات
البنزيل باستخدام طريقة الطي العكسي

عزت طه محمد سليم و محمد عبدالفتاح ربيع و مجدي الدين فهمي أحمد

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تم في هـذا البحـث دراسة عمليـات التأين في جـزيئـات الكحـول البنـزيلي والامين البنزيلي والسيانيـد البنزيلي لتكوين الايـون الاساسي للجزيئات الثلاثة بأستخدام تناطح الالكترونات مع جزيئات المركبـات الثلاثة بأستخدام مطيـاف الكتله طراز CH - 4 . ولقد تم قياس طاقـات التأين عنـد نقطة البدايـة لمنحنيـات كفاءة التأين بعد معالجتهـا بأستخدام طريقـة الطي العكسي (DFD) وهي ٨,٢٦ الكترون ڤولت للكحول البنزيلي، ٨,٤٩ الكترون ڤولت للامين البنزيلي، ٩,٣٢ الكترون ڤولت للسياند البنزيلي . وقـد أمكن تفسيـر عمليـة التأين عـلى أنها نتيجة لنزع أحد الالكترونات الاقل تماسكاً في رابطة الـ π لحلقة البنزيل ويرجع أختلاف قيم طاقة التأين لتأثير المجموعات المختلفة المضافة لحلقة البنزيل وقـد أمكن قياس طاقـات التأين لمستويات الطاقة الاعلى لكل أيون من خلال منحنيات كفاءة التأين والتي تم قياسها لمدى ٤ إلكترون ڤولت، وقد قام الباحثون بتفسير بعض مستويات الطاقة العليا التي تظهر في منحنيات كفاءة التأين للجزيئات الاسـاسية ومقارنتها بالايون الام (البنزيل)، وكذلـك أمكن مقارنـة بعض مستويـات الطاقـة المقاسه بمثيلاتها المقاسه بطرق أخرى .

وفي هذه الدراسة أيضاً أمكن قياس الطيف الكتلي لجزيئات الكحول البنزيلي والامين البنزيلي والسياند البنزيلي عند طاقتي ٧٠ ، ١٤ الكترون ڤولت، وقد تم دراسة تأثير مجموعات الهيدروكسيل (أيد) والامـين (ن يد ٢) والسيـانيد (ك ن) في

جـزيئي البنزيـل (ك٦ يده ك يـدر) على الـطيف الكتلي وكـذلك عنـد الـطاقـات المختلفة وأمكن مقارنـة نسب تكوين الايـونات الاسـاسية والايـونات الفـرعيه في الطيف الكتلي لهذه الجزيئـات الثلاثـة، وكذلـك تم دراسة ميكـانيكية تكسـير كل أيون جزيئي من الايونات الثلاثة في وجود المجموعات المختلفة.