

[TP] The mass spectrum of ethane, C_2H_6, has peaks at m/z = 14, 15, 27, 28, 29, and 30.
The peak with the highest relative intensity is at m/z = 28, and the peak with the lowest relative intensity is at m/z = 14. Which peak is due to the molecular ion?

13% 1. The peak at m/z = 14
13% 2. The peak at m/z = 15
13% 3. The peak at m/z = 27
13% 4. The peak at m/z = 28
13% 5. The peak at m/z = 29
13% 6. The peak at m/z = 30
13% 7. None of the above
13% 8. All of the above

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Lecture 5 CH101 A1 (MWF 9 am)

Friday, September 16, 2016

For today ...

- Molecular mass spectra

Next lecture: Mass spectra of compounds with Br (or Cl). Light, wavelength, frequency, and wavenumber; IR spectra

Memorize: Figs 3.19 (p75) and 3.24 (p 80)
Do not memorize: Table 3.5 (p 78)

Molecular mass spectra

Sketch mass spectrum of ethane, C_2H_6

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13% 6. The peak at m/z = 30
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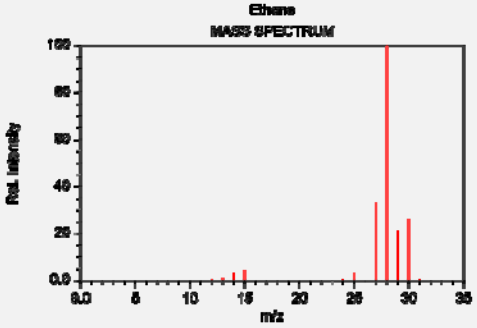
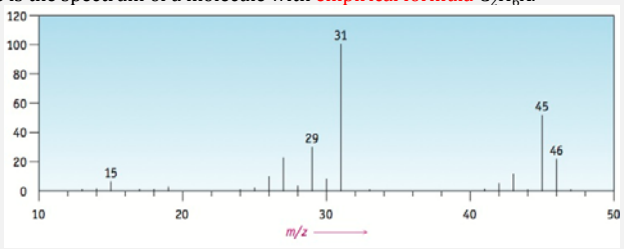
Sketch mass spectrum of ethane



Use the molecular ion to analyze mass spectrum

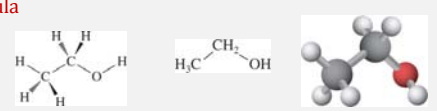
Here is the spectrum of a molecule with empirical formula C_2H_6X.

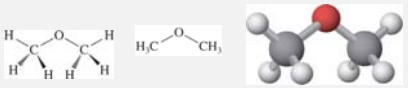


What element is X?

Important terms to distinguish

- Constitutional isomers: Ethanol and dimethyl ether
- Empirical formula: C_2H_6O
- Condensed formula: CH_3CH_2OH and CH_3OCH_3
- Structural formula

Ethanol: 

Dimethyl ether: 

[TP] Ethanol, CH_3CH_2OH,and dimethyl ether, CH_3OCH_3, are constitutional isomers. This means that their mass spectra ...

20% 1. must have the same molecular ion peak
20% 2. must contain the same number of peaks at the same places (m/z), but with different heights
20% 3. must contain the same number of peaks but at different places (m/z)
20% 4. 1 and 2
20% 5. 1 and 3

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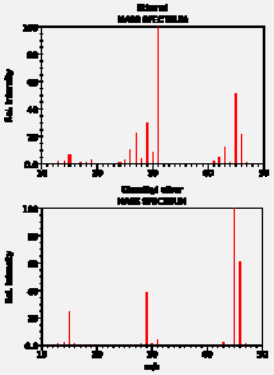
Ethanol and dimethyl ether, $C_2H_6O^+$



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Important isotopes (Table 3.4, p 68)

Element	Isotope	Relative Abundance	Exact Mass	Isotope	Relative Abundance	Exact Mass
carbon	^{12}C	98.90%	12.00000	^{13}C	1.10%	13.00335
oxygen	^{16}O	99.76%	15.99491	^{18}O	0.20%	17.99916
nitrogen	^{14}N	99.63%	14.00307	^{15}N	0.37%	15.00011
hydrogen	^{1}H	99.99%	1.00783	^{2}H	0.01%	2.01410
chlorine	^{35}Cl	75.78%	34.968852	^{37}Cl	24.20%	36.965902
bromine	^{79}Br	50.69%	78.918337	^{81}Br	49.31%	80.916291

C, O, N and H each have a one important isotope
F has one important isotope
Cl has two important isotopes: ^{35}Cl : ^{37}Cl :: 3:1
Br has two important isotopes: ^{79}Br : ^{81}Br :: 1:1

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