

[TP] Which of
CH_4, CH_3Br, and CH_2Br_2
has the greatest number of molecular ion peaks?

20% 1. CH_4
20% 2. CH_3Br
20% 3. CH_2Br_2
20% 4. CH_3Br and CH_2Br_2
20% 5. They each have the same number of molecular ion peaks

Response Counter 10

Lecture 6 CH101 A1 (MWF 9:05 am)

Monday, September 17, 2018

- Review: Molecular mass spectra
- Mass spectra of compounds with Br (or Cl)
- What is light

Next lecture: Jiggling of bonded atoms; Wavelength, frequency, and wavenumber; Infrared (IR) spectra
http://quantum.bu.edu/CDF/101/IRFrequency.cdf

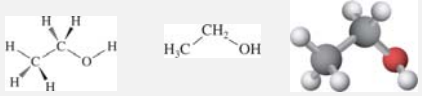
Memorize: Figs 3.19 (p75) and 3.24 (p 80)
Do not memorize: Table 3.5 (p 78)

Representative questions: On IR: 3.25, 3.59, 3.61,

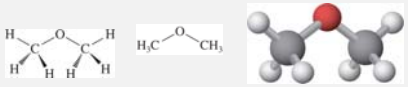
Important terms to distinguish

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

Ethanol:

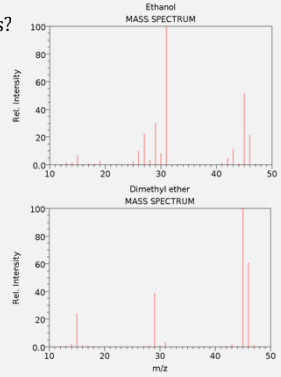


Dimethyl ether:



Ethanol and dimethyl ether, $C_2H_6O^+$

What are the fragments?



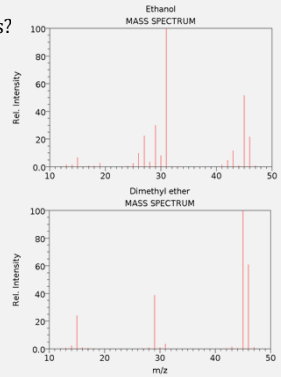
[Quiz] Ethanol, CH_3CH_2OH, has peaks at m/z = 25, 26, 27, and 28, but dimethyl ether, CH_3OCH_3, does not. A reason for this could be that …

20% 1. ethanol does not have O bonded to C
20% 2. dimethyl ether does not have O bonded to C
20% 3. dimethyl ether does not have C bonded to C but ethanol does
20% 4. dimethyl ether does not have H bonded to O
20% 5. dimethyl ether has C-O-C bonds but ethanol does not

Response Counter 10

Ethanol and dimethyl ether, $C_2H_6O^+$

What are the fragments?



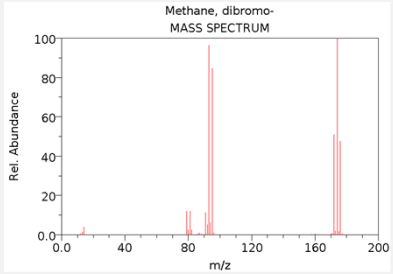
Mass spectra of compounds with Br (or Cl)

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

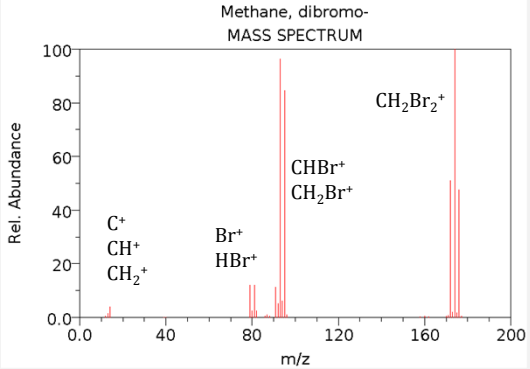
CH_2Br_2 mass spectrum



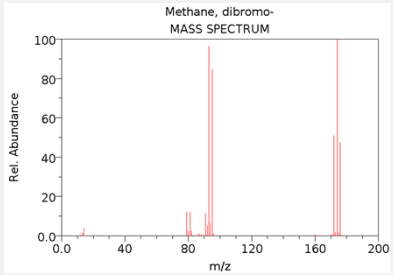
What accounts for each of these singly-charged ion peaks?

Peaks at largest m/z always due to molecular ion, here $CH_2Br_2^+$

CH_2Br_2 mass spectrum



CH_2Br_2 mass spectrum



	^{79}Br ½	^{81}Br ½
^{79}Br ½	½ x ½ = ¼	½ x ½ = ¼
^{81}Br ½	½ x ½ = ¼	½ x ½ = ¼

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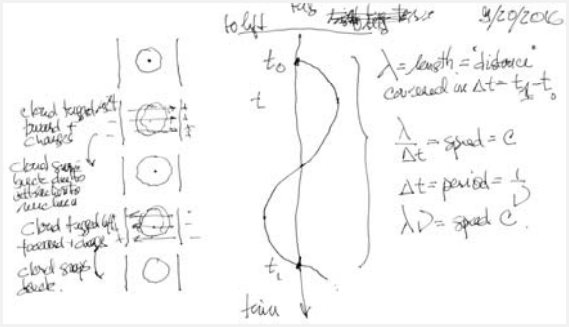

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