

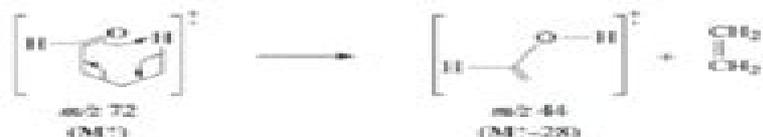
Mass Spectrometry: PART 2

some solved problems

Question 1

- A compound with molecular formula C_4H_8O has a strong IR adsorption at 1730 cm^{-1} . Its mass spectrum includes key peaks at m/z 44 (the base peak) and m/z 29. Propose a structure and write fragmentation equations showing how these peaks are formed.

Answer: the compound is butanal. The peak at m/z 44 arises from a McLafferty rearrangement (see next slide for an example). This rearrangement happens to carbonyl compounds that have a hydrogen on their alpha carbon.



The peak at m/z 29 arises from a fragmentation producing an acylium ion.



✧ Ketones

● McLafferty rearrangement



Mass Spectroscopy Problems And Solutions

Wade A. Freeman



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