

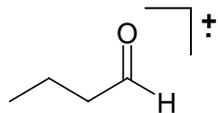
Problem Set 5. April 5, 2007.

Mass Spectrometry

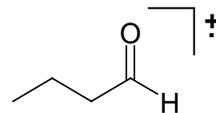
CHEM393

Dr. H.M. Muchall

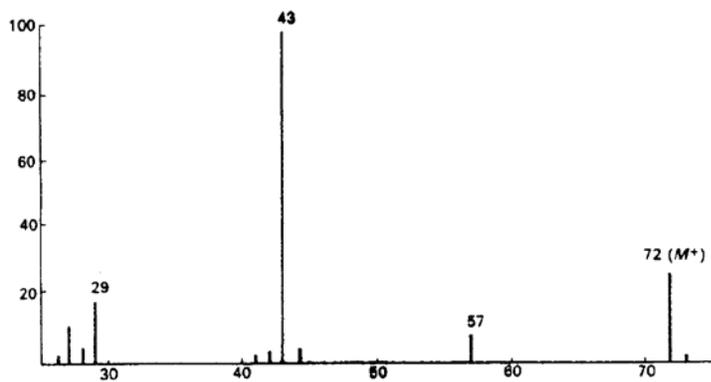
1. (5 points) For the butanal with signals in the mass spectrum at m/z 72, 57, 44, 43, 41 and 29, show (put + and · on the more likely species)



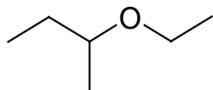
- b) a McLafferty rearrangement (both fragments).



2. (6 points) Give the species from the fragmentations (labeled masses) in the mass spectrum of butanone. Make sure you indicate radical cations, cations or radicals where appropriate. Include the masses of all fragments in the scheme.



3. The ether below shows a fragmentation m/z 102 \rightarrow 87. Three pathways are possible.



a) (6 points) Show all three possible fragmentations. Include all $+$, \cdot and masses. Which of these fragmentations is unlikely?

b) (4 points) Knowing that m/z 87 further fragments to give m/z 31 in an onium reaction, which of the two remaining fragments from a) do you pick? Show the fragments from the onium reaction.

4. (3 points) Which of the following shows correct retro-Diels-Alder fragments for the indicated compound? Which fragment carries the $+$ preferentially?

