

- 1) Predict the masses and the structures of the most abundant fragments observed in the mass spectra of the following compounds:
  - a) 2-methylpentane
  
  
  
  
  
  
  
  
  
  
  - b) 3-methyl-2-hexene
  
  
  
  
  
  
  
  
  
  
  - c) 4-methyl-2-pentanol
  
- 2) Give logical fragmentation to account for the following ions observed in these mass spectra.
  - a) n-octane: 114, 85, 71, 57
  
  
  
  
  
  
  
  
  
  
  - b) methylcyclohexane: 98, 83
  
  
  
  
  
  
  
  
  
  
  - c) 2-methyl-2-pentene: 84, 69
  
  
  
  
  
  
  
  
  
  
  - d) 1-pentanol: 70, 55, 41, 31
  
- 3) The mass spectrum of n-octane shows a prominent molecular ion peak at 114. There is also a large peak at 57 but is not the base peak. The mass spectrum of 3,4-dimethylhexane shows a smaller molecular ion, and the peak at mass 57 is the base peak. Explain these trends in abundance of the molecular ions and the ions at mass 57, and predict the intensities of the peaks at masses 57 and 114 in the spectrum of 2,2,3,3-tetramethylbutane.

- 4) An unknown, foul smelling hydrocarbon gives the mass spectrum and infrared spectrum shown below.
- Use the mass spectrum to propose a molecular formula. How many degrees of unsaturation are there?
  - Use the IR spectrum to determine any functional groups present.
  - Propose one or more structures for this compound. What parts of the structures are uncertain? If you knew that the hydrogenation of this compound gives n-octane, would the structure still be uncertain?
  - Propose the structures for the major fragments at 39, 67, 81 and 95 in the mass spectrum. Explain why the base peak is so strong.

