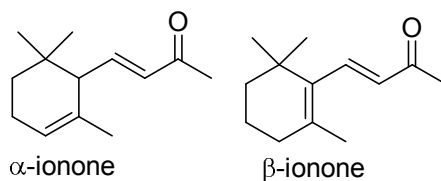
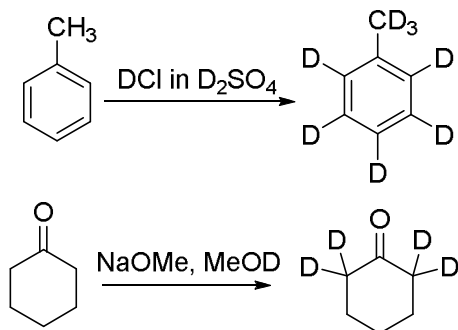


#### Assignment 4 – Mass spectrometry

1. What should be the minimum resolution of a mass spectrometer that can distinguish ethylhydrazine ( $\text{CH}_3\text{CH}_2\text{NHNH}_2$ ) from 2-hydroxyacetaldehyde ( $\text{HOCH}_2\text{CHO}$ ) based on their high resolution mass spectral data to 5 decimal places? (mass C = 12.0000, H = 1.00783, N, 14.0031 and O = 15.9949). (5 marks)
2. In the molecular ion region how many isotope peaks will be seen in the mass spectrum of 2,3-dichloro-1-bromopropane? What are their relative intensities? (5 marks)
3. Mass spectrum of limonene gives a fragment peak at  $m/z$  68 which is half the  $m/z$  value of the molecular ion peak. Write a suitable fragmentation mechanism of limonene that accounts for the peak at  $m/z$  68. What is the name of the fragmentation process? (5 marks)
4. The structure of  $\alpha$ -ionone and  $\beta$ -ionone are shown below. Mass spectrum of one of the isomers gave base peak at  $m/z$  177 while the other isomer gave base peak at  $m/z$  136. Assign which one is which and account for the fragmentation processes responsible for these peaks. (5 marks)

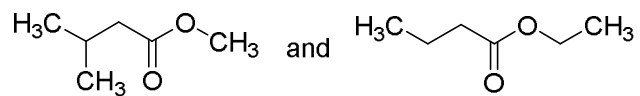


5. Mass spectrum of *n*-butylbenzene gave two peaks at  $m/z$  92 (60%) and  $m/z$  91 (100). Write fragmentation process from the molecular ion that would account for these fragment ions. (5 marks)
6. The following reactions were separately monitored by examining aliquots of sample drawn periodically from the reaction mixtures and analyzing the same by mass spectrometry. How can MS ensure completion of the reaction? (5 marks)

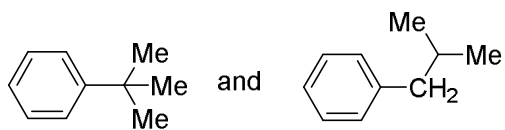


7. How can the following pairs of isomers be distinguished by mass spectrometry. Discuss key distinguishing features of the spectrum for each one in the pair. (5 x 4 = 20 marks)

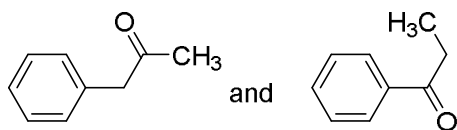
(a)



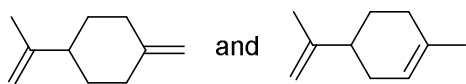
(b)



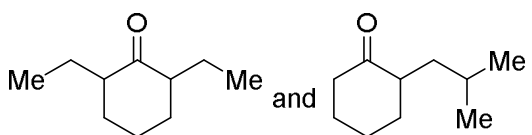
(c)



(d)



(e)



END