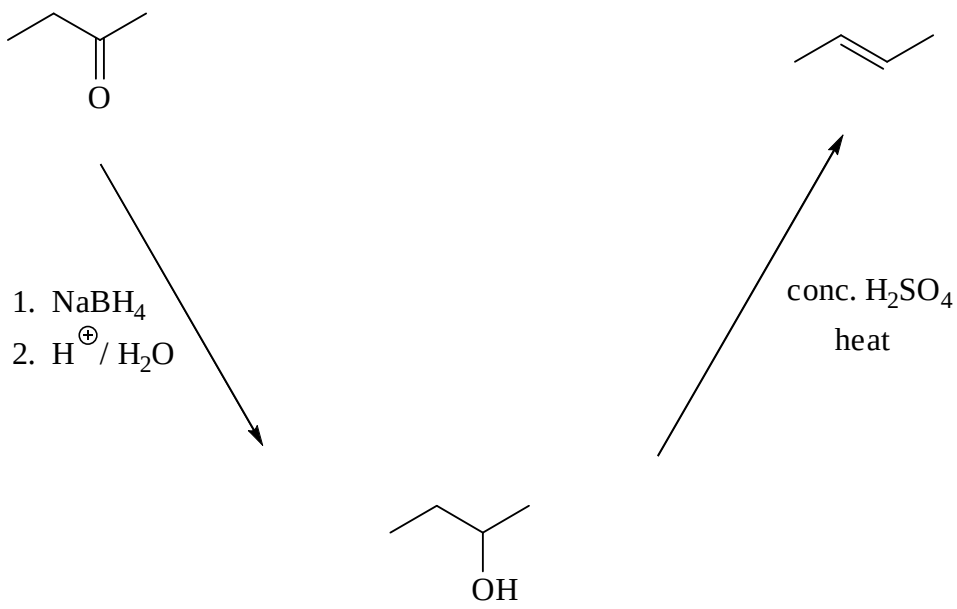
Marks 8

- Show clearly the reagents you would use to carry out the following chemical conversion. Two steps are required. Give the structure of the intermediate compound.



How can IR spectroscopy distinguish between the starting material, the intermediate and the product?

The starting material absorbs strongly in the 1650-1800 cm^{-1} region due to the presence of the carbonyl (C=O) group.

The intermediate absorbs strongly in the 3000-3300 cm^{-1} region due to the presence of the alcohol (O-H) group .

The product does not absorb strongly in either of these regions.

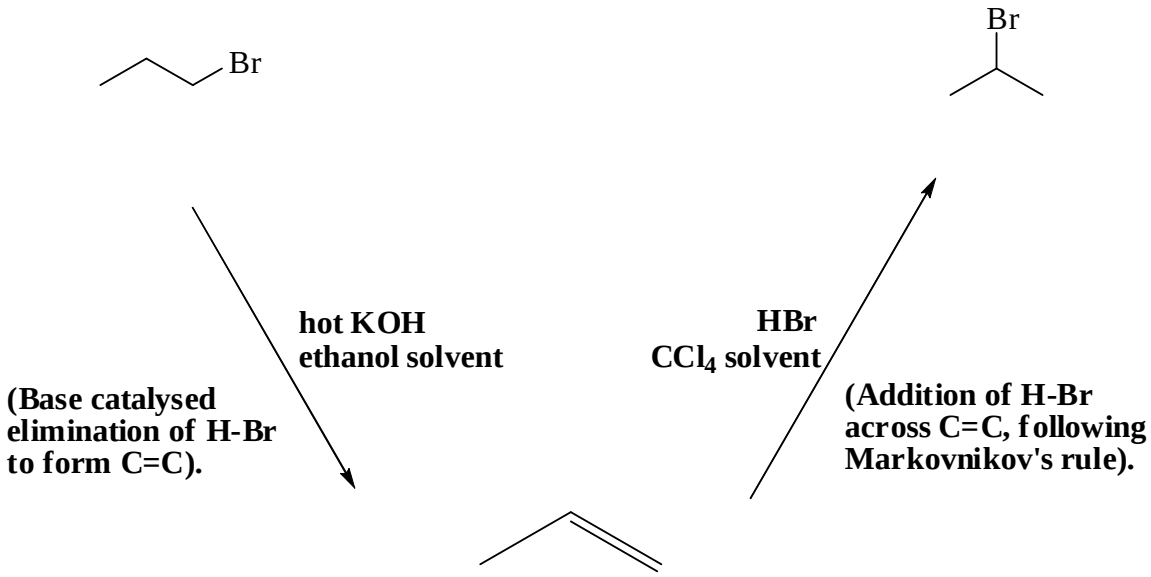
How can ^{13}C NMR spectroscopy distinguish between the starting material, the intermediate and the product?

The product is symmetrical and has only 2 resonances.

The starting material and the intermediate both have 4 resonances, but the chemical shifts will differ: the carbonyl C in the starting material is at higher chemical shift (180-200 ppm) than the C–OH carbon (~50 ppm).

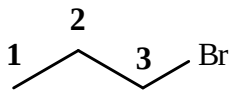
Marks 5

- Show clearly the reagents you would use to carry out the following chemical conversion. Two steps are required. Give the structure of the intermediate compound.

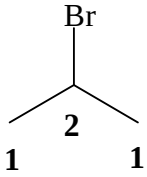


How could you distinguish between the starting material and the product by ^{13}C NMR spectroscopy?

The starting material has 3 different carbon environments so will give 3 resonances in the ^{13}C NMR.



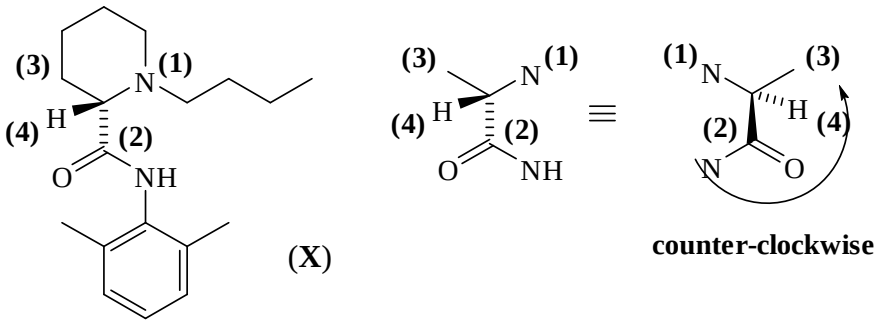
The produt has 2 different carbon environments so will give 2 resonances in the ^{13}C NMR.



The two carbon atoms labelled as '1' are equivalent.

Marks 7

- Bupivacaine is the active molecule in some local anaesthetics. Of the two enantiomers, the one shown below (**X**) is the more effective.



What is the molecular formula of (**X**)?

$C_{18}H_{28}ON_2$

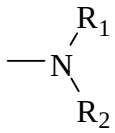
Calculate the *m*/*z* value for the major peak you would expect to see for the molecular ion in the high resolution mass spectrum.
[Atomic masses: $^{1}H = 1.0078$; $^{12}C = 12.0000$; $^{16}O = 15.9949$; $^{14}N = 14.0031$]

The molecular ion has *m* = molar mass:

Molar mass = (18 × 12.0000 (C) + 28 × 1.0078 (H)
+ 15.9949 (O) + 2 × 14.0031 (N)) g mol^{-1} = 288.2195 g mol^{-1}

Answer: **288.2195 g mol^{-1}**

List the substituents attached to the stereogenic centre in descending order of priority according to the sequence rule.

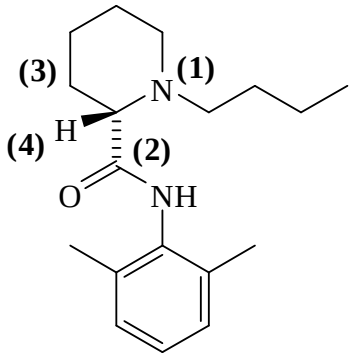
highest priority			lowest priority
	—CONHR	—CH_2—	—H

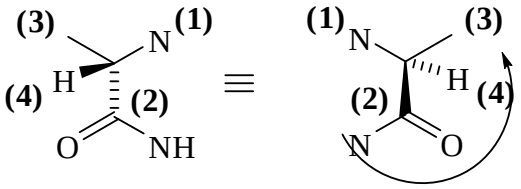
What is the absolute stereochemistry of **(X)**? Write (*R*) or (*S*).

(*S*)
(see above)

Name the functional groups present in (**X**).

(tertiary) amine, amide, aromatic ring





counter-clockwise